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# Optimisation-based Methodology for the Design and Operation of Sustainable Wastewater Treatment Facilities

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## Declaration of Originality

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Channarong Puchongkawarin
October 2015

# Abstract

The treatment of municipal and industrial wastewaters in conventional wastewater treatment plants (WWTPs) requires a significant amount of energy in order to meet ever more stringent discharge regulations. However, the wastewater treatment industry is undergoing a paradigm shift from a focus on waste-stream treatment and contaminant removal to a proactive interest in energy and resource recovery facilities, driven by both economic and environmental incentives. The main objective of this thesis is the development of a decision-making tool in order to identify improvement opportunities in existing WWTPs and to develop new concepts of sustainable wastewater treatment/recovery facilities.

The first part of the thesis presents the application of a model-based methodology based on systematic optimisation for improved understanding of the tight interplay between effluent quality, energy use, and fugitive emissions in existing WWTPs. Plant-wide models are developed and calibrated in an objective to predict the performance of two conventional activated sludge plants owned and operated by Sydney Water, Australia. In the first plant, a simulation-based approach is applied to quantify the effect of key operating variables on the effluent quality, energy use, and fugitive emissions. The results show potential for reduced consumption of energy (up to 10-20%) through operational changes only, without compromising effluent quality. It is also found that nitrate (and hence total nitrogen) discharge could be signficantly reduced from its current level with a small increase in energy consumption. These results are also compared to an upgraded plant with reverse osmosis in terms of energy consumption and greenhouse gas emissions. In the second plant, a systematic model-based optimisation approach is applied to investigate the effect of key discharge constraints on the net power consumption. The results show a potential for reduction of energy (20-25%), without compromising the current effluent quality. The nitrate discharge could be reduced from its current level to less than 15 mg/L with no increase in net power consumption and could be further reduced to <5 mg/L subject to a 18% increase in net power consumption upon the addition of an external carbon source. This improved understanding of the relationship between nutrient removal and energy use for these two plants will feed into discussions with environmental regulators regarding nutrient discharge licensing.

The second part of the thesis deals with the application of a systematic, model-based methodology for the development of wastewater treatment/resource recovery systems that are both economically and environmentally sustainable. With the array of available treatment and recovery options growing steadily, a superstructure modeling approach based on rigorous mathematical optimisation provides a natural approach for tackling these problems. The development of reliable, yet simple, performance and cost models is a key issue with this approach in order to allow for a reliable solution based on global optimisation. it is argued that commercial wastewater simulators can be used to derive such models. The superstructure modeling framework is also able to account for wastewater and sludge treatment in an integrated system and to incorporate LCA with multi-objective optimisation to identify the inherent trade-off between multiple economic and environmental objectives. This approach is illustrated with two case studies of resource recovery from industrial and municipal wastewaters. The results establish that the proposed methodology is computationally tractable, thereby supporting its application as a decision support system for selection of promising wastewater treatment/resource recovery systems whose development is worth pursuing. Our analysis also suggests that accounting for LCA considerations early on in the design process may lead to dramatic changes in the configuration of future wastewater treatment/recovery facilities.

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# List of Publications

### Peer-reviewed Publications

C. Puchongkawarin, C.Menichini, C. Laso-Rubido, S. Fitzgerald, B. Chachuat. Model-based methodology for plant-wide analysis wastewater treatment plant of WWTPs: a case study. *Water Practice and Technology*, 10(3):517-526, 2015.

C. Puchongkawarin, C. Gomez-Mont, D.C. Stuckey and B. Chachuat. Optimization-based methodology for the development of wastewater facilities for energy nutrient recovery. *Chemosphere*, 140:150-158, 2015.

C. Puchongkawarin, Y. Vaupel, G. Miao, N. Shah, D. Stuckey, B. Chachuat, Incorporation of LCA into the systematic synthesis of wastewater treatment plants (Preparation).

C. Puchongkawarin, S. Fitzgerald, B. Chachuat, Plant-wide optimization of a full-scale activated sludge plant with anaerobic sludge treatment (Preparation).

### Chapters in Books

C. Puchongkawarin, Y. Vaupel, G. Miao, N. Shah, D. Stuckey, B. Chachuat, Towards the synthesis of wastewater recovery facilities using enviroeconomic optimization (Submitted).

### Papers in Peer-Reviewed Conference Proceedings

C. Puchongkawarin, S. Fitzgerald, B. Chachuat. Plant-wide optimization of a full-scale activated sludge plant with anaerobic sludge treatment. In 9th IFAC Symposium on Advanced Control of Chemical Processes, Whistler, Canada, 2015.

### Presentations at Conferences

C. Puchongkawarin, Y. Vaupel, G. Miao, N. Shah, D. Stuckey, B. Chachuat, Incorporation of LCA into the systematic synthesis of wastewater treatment plants. In Energy and water security, Doha, Qatar, 2015.

C. Puchongkawarin, C. Menichini, C. Laso-Rubido, S. Fitzgerald, B. Chachuat, Towards a new understanding of the balance between energy use and effluent quality. In Enviro14, Adelaide, Australia, 2014.

C. Puchongkawarin, C. Menichini, C. Laso-Rubido, S. Fitzgerald, B. Chachuat, Model-based methodology for plantwide optimization of WWTPs: A case study. In 2nd IWA Specialist Conference on EcoTechnologies for Sewage Treatment Plants, Verona, Italy, 2014.

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**Technical Reports**

C. Puchongkawarin, Optimisation modelling of energy and effluent, Technical Report for Sydney Water 2014.

# List of Abbreviations

| | |
|---|---|
| A2O | Anaerobic Anoxic Aerobic process for |
| ADM1 | Anaerobic Digestion Model No. 1 |
| AFMBR | Anaerobic Fluidized Membrane Bioreactor |
| AOB | Ammonia Oxydizing Bacteria |
| ASDM | Activated Sludge Digestion Model |
| ASM1 | Activated Sludge Model No. 1 |
| ASM2 | Activated Sludge Model No. 2 |
| ASM2d | Activated Sludge Model No. 2d |
| ASM3 | Activated Sludge Model No. 3 |
| BNR | Biological Nitrogen Removal |
| BOD | Biochemical Oxygen Demand |
| BSM1 | Benchmark Simulation Model No. 1 |
| BSM2 | Benchmark Simulation Model No. 2 |
| CCA | Climate Change Act |
| CHP | Combined Heat and Power |

| | |
|---|---|
| COD | Chemical Oxygen Demand |
| DAF | Dissolved Air Flotation |
| DO | Dissolved Oxygen |
| EPA | Environment Protection Authority |
| EQI | Effluent Quality Indicator |
| GAMS | General Algebraic Modeling System |
| GHG | Greenhouse Gas |
| GWP | Global Warming Potential |
| HRT | Hydraulic Retention Time |
| HTAL | Hydrotalcite |
| IWA | International Water Association |
| LCFA | Long Chain Fatty Acid |
| MBBR | Moving Bed Biofilm Reactor |
| MBR | Membrane Bioreactor |
| MINLP | Mixed-integer Nonlinear Programming |
| MLE | Modified Ludzack Ettinger |
| MLR | Mixed Liquor Recycle |
| MLSS | Mixed Liquor Suspended Solids |
| NOB | Nitrite Oxidizer Bacteria |
| NPV | Net Presetn Value |
| OCI | Operational Cost Indicator |

| | |
|---|---|
| PAO | Phosphorus Accumulating Organism |
| PE | Population Equivalent |
| PHA | Polyhydroxyalkanoates |
| PID | Proportional Integral Derivative |
| PPCPs | Pharmaceutical and Personal Care Products |
| RAS | Return Activated Sludge |
| RO | Reverse Osmosis |
| SAnMBR | Submerged Anaerobic Membrane Bioreactor |
| SCE | Solid Capture Efficiency |
| SHARON | Single Reactor High Activity Ammonium Removal over Nitrite |
| SRT | Solid Retention Time |
| TN | Total Nitrogen |
| TP | Total Phosphorus |
| TSS | Total Suspended Solid |
| UASB | Upflow Anaerobic Sludge Blanket |
| UK | United Kingdom |
| UN | United Nation |
| VFA | Volatile Fatty Acid |
| VFD | Variable Frequency Drive |
| WAS | Waste Activated Sludge |
| WDS | Water Distribution System |

| | |
|---|---|
| WFD | Water Framework Directive |
| WWTP | Wastewater Treatment Plant |

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# Chapter 1

# Introduction

As the world's population is expected to reach over 8 billion by 2030, the global challenge for humanity is to cope with growing demands for water, energy and food in the face of increasingly scarce resources. The U.N. estimates that we will need 30% more water, 45% more energy and 50% more food by 2030, and climate change will exacerbate this situation even further [1]. Water, energy and food are inextricably interconnected and considered as the water-food-energy nexus (Figure 1.1). Globally, 70% of freshwater is used for the agricultural sector in terms of agricultural production, forestry, fisheries and the agri-food supply chain, making it the first water consumer [2]. Large quantities of water are also needed in most power generation processes, including electricity, hydropower and cooling for thermal power. At the same time, food production and its supply chain uses 30% of the energy consumed globally [3], and energy is used to extract, lift, pump, transport and treat water. In this context, growing demands for water, energy and food, and increasing competition for resources between them, may affect livelihoods and the environment in unpredictable ways.

The water-energy-food nexus is regarded as a system governed by complexity and interconnections that cannot be accounted for separately. A sudden change in one aspect can cause unpredicted and dangerous outcomes. In an irrigated agricultural sector, for example, growing bioenergy crops can potentially increase energy supply and employment opportunities, but this may lead to problems regarding land use and water resources [4]. To date, a system-wide method of considering these three aspects is not widely understood and rarely used in decision-making policy and regulation because the existing water-energy-food policies are developed in isolation from each other. As a result, there are negative consequences in terms of economic, environmental and social aspects such as commodity prices, sub-optimal infrastructure design, as well as environmental degradation. An important step toward integration of the energy-water-food nexus is to develop an analytical tool, conceptual model, appropriate validation method and data set that can provide insights into the future of energy, water and food [5]. In addition, climate change has already started to affect precipitation and temperature patterns, as well as population growth continuing to increase. All these factors may have large impacts on the management of food, energy and water systems.

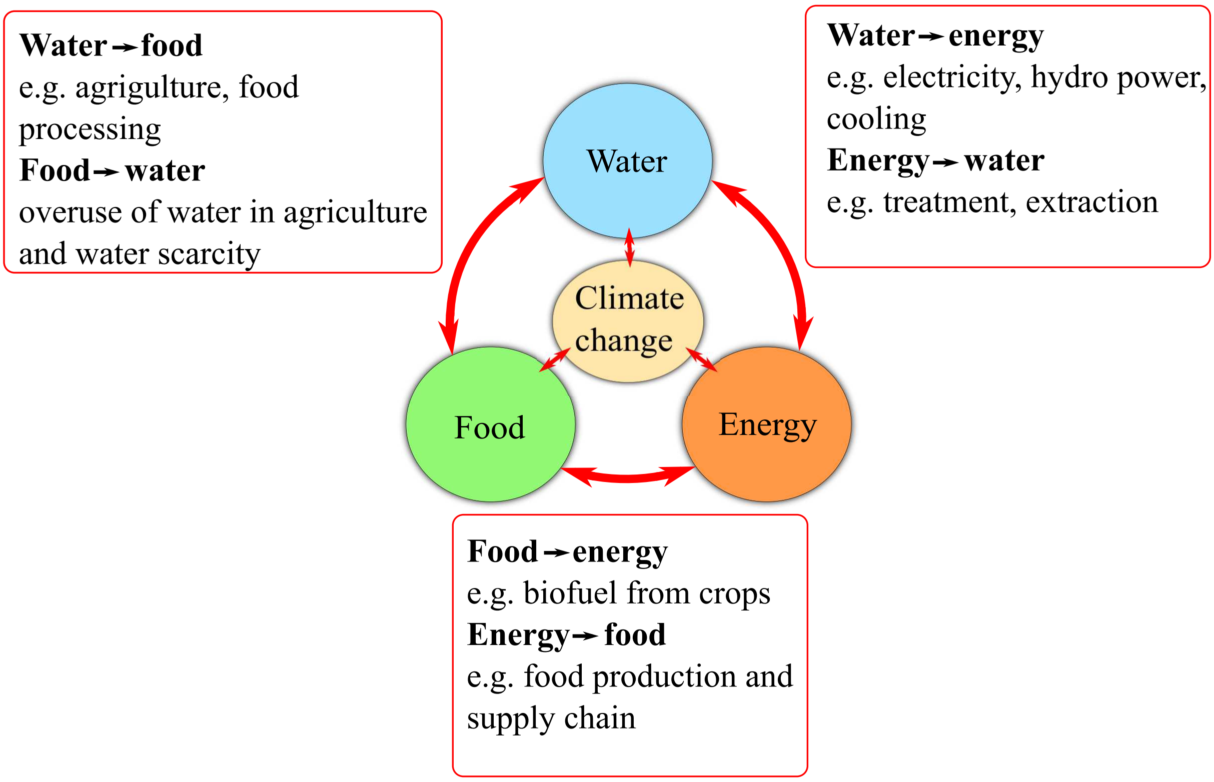



Figure 1.1: Water energy food nexus.

## 1.1 Wastewater Treatment Challenges

Wastewater treatment plants (WWTPs) have played an important role in returning clean and safe water back to the environment, and are regarded as a portion of the broader nexus between water and energy [6]. Every step in the WWTP requires energy, from wastewater collection to discharge, meanwhile the treated water can be reused for generating energy. To produce satisfactory effluent quality for discharge into the environment, wastewater treatment processes require large amount of energy, mostly as electricity, which is likely to increase in the future due to increasing population and stricter discharge regulations. In the UK, for example, there are around 9,000 operating WWTPs [7], consuming around 1% of the overall electricity demand in the UK for treating sewage wastewater; this makes it the fourth most energy intensive sector in the UK economy. In an aim to continuously improve surface water quality, it is likely that effluent regulations will be tightened in the future, along with an increasing population, which will increase the energy footprint of WWTPs even further. This higher energy consumption will have a negative impact on the global water industry, and is inextricably connected to climate change because electrical energy, the main energy source in the WWTPs, is produced from fossil fuels. These are becoming major concerns for the WWTP industry in terms of progressing towards economic viability and environmental sustainability simultaneously.

In addition, a major challenge for WWTPs is disposing of the sludge produced in the WWTPs. There are several problems associated with this sludge, such as an increase in sludge production, increasing costs for sludge treatment, and the risks of sludge to the environment and to human health. This is because toxic contaminants including pathogens in wastewater are concentrated in the sludge. Awareness of the risks associated with sludge to the environment and human health has increasingly affected sludge application as fertilizers in the agricultural sector. Policy and regulations associated with sludge treatment and disposal have been developed to control the adverse impact of toxic pollutants and pathogens. These have led to increased pressures for wastewater treatment design and operation to achieve sustainability.

Sustainability is normally defined by the World Commission on Environment and Development on the sustainability development as "*Development that meets the needs of the present generations to meet their own needs*" [8]. However, this is a fundamental concept rather than an exact meaning so its definition can be subjective and change from time to time. Mitcham [9] made the criticism that sustainability could mean almost anything. Instead, sustainability is typically defined in three dimensions in terms of economic, environmental and social cultural [10].

- Economic sustainability - This focuses on an increase of human quality of life to meet and satisfy human needs. The utilities should be financially viable with sufficient resources to maintain their infrastructure.
- Environmental sustainability - It should be an energy neutral system with minimal chemical consumption. Nutrient management should be performed to minimise dispersal to the aquatic environment. Also, the wastewater industry has to minimise the other environmental impacts regarding air pollutions (e.g. $CO_2$, $N_2O$ and $CH_4$) and other impacts from energy and chemical use.
- Social-cultural sustainability - This aspect may have different definitions for different people. People are aimed to have equally social-cultural and spiritual with stable morality, relationships and institutions [10].

In the wastewater treatment community, these aspects of sustainability and key factors contributing to sustainable wastewater treatment facilities are investigated using different tools, e.g. economic analysis and life cycle assessment (LCA) as a single or multiple indicators. The assessment of sustainability by using these indicators is well-established and found in many studies [10, 11]. It is noted that selection of the indicators varied from study to study which depends on geography, culture, and population served [12]. More specifically, sustainability in this study focuses on economic and environmental sustainability which aims to maximise human quality of life to satisfy needs and minimisation of the overall environmental impacts. The financial indicator in terms of the net present value (NPV) and the LCA methodology would be used to quantify economic and environmental sustainability. The social-cultural sustainability is not considered in this study because there is no standard approach to evaluate the social sustainability [13].

Achieving economic and environmental sustainability of wastewater treatment processes can be performed through either improvement of existing WWTPs or construction of new wastewater treatment facilities. The former can be accomplished in the short-to-medium period of time compared to the latter. Over the last few decades, pollution reduction measures on the quality of water bodies have been set as the first priority for wastewater treatment processes. An improvement in effluent quality to minimise contaminants, such as lower levels of COD or nutrients, typically requires more intensive treatment, which often entails larger energy consumption. To address this issue, the development of improved operational and control strategies is a promising option among alternatives for the sewage industry because it involves a reduction in energy required, and an improvement in effluent quality, which may not require any cost in terms of further investment [14]. However, it is not a straight-forward task because wastewater influent varies substantially from one place to another, a variety of biological processes, e.g. activated sludge and anaerobic digestion acting on different time scale and interacting with each other through recycle streams. This has driven decision-makers to use modeling techniques to improve plant operation. Mathematical modeling of WWTPs has become increasingly accepted as a tool for practical use as it can provide reliable predictions of a plant's behavior by capturing the major process dynamics thereof, and is used to predict reliable behaviour of the system. An important hurdle to the widespread application of such models for WWTPs is to develop reliable models despite the limited amount of information that is typically available (lack of characterization of the incoming wastewater and at different stages of the treatment). Despite carrying significant uncertainty, models can still provide valuable insights in assessing and comparing different control and operational strategies.

Parallel to the improvement of existing WWTPs, development of new wastewater treatment facilities is equally important to achieve sustainability. Most wastewater treatment plant design is still similar to when it was established back in the early $20^{th}$ century [15]. While the primary aim of conventional WWTPs is to protect human health and the environment, they are becoming one of the largest energy consumers in the UK. Evaluation of the sustainability of WWTPs has been carried out in the the past 15 years, and the goal of WWTPs should go beyond wastewater purification. A paradigm shift is currently under way towards making WWTPs more sustainable; in the new paradigm, wastewater is regarded as a renewable resource from which water, energy and materials can be recovered by using resource recovery facilities [16]. Resource recovery from wastewater requires not only the development of new technologies, but also decision making tools that help to evaluate innovative approaches on the basis of economic, environmental and social aspects. A challenge here is to select a combination of treatment/recovery technologies and interconnections among alternatives for treating a given wastewater influent (flowrate and concentrations) to achieve performance criteria while meeting effluent requirements. Currently, WWTP design is mostly based on design rules and guidelines e.g. Metcalf & Eddy [17] used by engineers, which is limited for the modern technologies or configurations due to a steady increase in degree-of-freedoms and objectives that need to be satisfied, e.g. effluent requirements, cost and safety. Complex WWTPs with a large number of treatment or separation units and interconnections require systematic optimisation tools [10, 18]. Superstructure optimisation [19] provides an ideal approach to identifying optimal solutions of complex design problems and it can account for multiple conflicting objectives, e.g. economic and environmental performance indicators. This approach has been increasingly applied to the synthesis of water networks [20, 21, 22, 23, 24], but only limited optimisation research have been reported on wastewater treatment and resource recovery systems [25, 26, 27, 28]. These studies provide insight into the potential of the systematic optimization-based approaches for wastewater treatment design, but they are nonetheless limited to optimizing a given process or selecting the most appropriate process among a small number of alternatives mainly based on economical considerations.

Because it is computationally demanding, the key to its success and novelty is the development and selection of mathematical models for the units that are simple enough for the optimisation problems to remain tractable, yet to provide reliable estimates of their process performances and associated cost and environmental indicators.

Overall, this thesis aims to develop decision-making tools to identify the optimal conditions for wastewater treatment design and operation using model-based methodology to achieve economic and environmental sustainability. With the wastewater treatment challenges above, applications of the model-based methodology can provide a better understanding of the link between economic and environmental aspects to improve operational strategies of existing WWTPs and valuable insights to select wastewater treatment/resource recovery facilities among process alternatives to achieve the performance targets, while meeting effluent discharge requirements. The developed decision-making tool can be expectedly used by a wide range of users including policy makers, plant managers, researchers, engineers, environmental regulators and operators. The users should have a basic knowledge of the system under study and aim to learn further about the economic and environmental implications of the tools. The research gaps and specific aims will be discussed in the next Chapter.

## 1.2 Outline of Thesis

The rest of the thesis is organized as follows. Chapter 2 surveys the literature on conventional WWTPs and their energy use; this includes common ways to improve the WWTP, and a model-based methodology for process optimisation and process design (a decision-making tool) to improve sustainability in WWTPs. Chapter 3 presents the application of a plant-wide model to evaluate operational strategies. In this chapter, a plant-wide model is developed and calibrated with data obtained from the full-scale WWTP owned and operated by Sydney Water to perform scenario analysis and improve operational strategies. Later, the application of a systematic optimisation for WWTPs is presented in Chapter 4, which also includes the model development, calibration and scenario analysis. Chapter 5 presents a systematic approach for the synthesis of WWTPs based on a superstructure optimisation-based approach. The use surrogate models in the optimisation formulation for model tractability is proposed. Also, the extended study for the synthesis of the WWTPs is presented by incorporating biosolids treatment and life cycle assessment in the optimisation problem in Chapter 6. Finally, Chapter 7 concludes with the main contributions of this thesis and discusses future research directions.

# Chapter 2

# Literature Review

Depletion of resources including fossil fuels and environmental pollution are the main driving forces for better wastewater treatment. While the elimination of contaminants in wastewater is an important task, sustainability is gradually becoming part of the criteria for decision makers during process design and operation. Conventional wastewater treatment processes are energy intensive, and considerable amounts of excess sludge and greenhouse gases (GHGs) such as $CO_2$ and $N_2O$ are produced and emited into the atmosphere during treatment. Consequently, they can have a negative impact on the environment and its ecology. Several studies have been carried out in order to address such problems which are likely to become worse in the near future. This literature review chapter covers the general background of the wastewater treatment processes, which includes the environmental impact of wastewater and conventional WWTPs. Also, typical problems regarding WWTPs, e.g. energy use and GHG emissions are discussed in order to investigate the opportunities to improve exising wastewater treatment facilities. Finally, several approaches towards sustainability will be discussed ranging from short (energy efficiency) to longer term (resource recovery) plans, including the use of modeling to solve energy and environment-related problems.

## 2.1 Wastewater and its Environmental Impacts

In the UK, over 11 billion litres of wastewater are treated daily by 9,000 sewage treatment facilities before discharge to inland waters, estuaries and the sea. Without appropriate treatment, wastewater can potentially damage the water environment and cause public health problems [7]. Wastewater contains organic matter, nutrients, bacteria and chemicals. The negative impacts of wastewater depend on the volume of wastewater, and the chemical and microorganisms concentrations/compostion [29]. Aerobic bacteria use dissolved oxygen in wastewater to degrade these substances, and when there are more bacteria, substrate, dissolved oxygen in wastewater becomes depleted, leading to anaerobic conditions which can produce maldorous gases and adverse impacts on aquatic life, and other undesirable consequences. Nutrients, especially nitrogen and phosphorus, are the primary constituents limiting the untrammelled growth of algae in the environment (eutrophication). The presence of these nutrients stimulates the growth or blooms of aquatic plants, e.g. algae,which limit light penetration, and can reduce their growth and cause these plants to die. When these plants eventually die, bacteria use dissolved oxygen in water to decompose the plants,which causes a reduction in oxygen in the water and affects the aquatic population. In addition, wastewater used for crop production or farming communities can also cause adverse impacts on communities and ecosystems. For instance, when nutrients leach down through the soil, they can potentially degrade groundwater quality [30]. Problems regarding wastewater are becoming increasingly difficult to handle because of rapidly increasing populations, and extensive industrialization. Wastewater generated from domestic activities and/or industrial processes can be a major source of pollution, consisting of a wide range of chemical contaminants and microorganisms.

Currently, there are several key indicators of water quality, e.g. biological oxygen demand (BOD), chemical oxygen demand (COD), dissolved oxygen (DO), suspended solids, ammonia nitrogen, nitrate, nitrite, phosphate and other nutrients, as well as trace metals. There are also emerging pollutants such as pharmaceutical and personal care products

(PPCPs) released in the wastewater [31]. High concentrations of these pollutants, except dissolved oxygen, above the regulated values are unacceptable in water receiving bodies due to their negative impacts on the environment, and health impacts on humans and animals. Wastewater treatment is required to remove organic matter, nutrients and toxic metals to acceptable levels before discharge and reuse. Standard regulations set by the environmental regulators specify the amount and concentrations of wastewater that are allowed to be discharged. Failure to meet such standards can result in heavy fines, or further punishment. Over the past 40 years, regulatory standards for wastewater discharge have become more and more important for improving water quality. In an attempt to improve water quality in the UK and Europe, the EU Water Framework Directive was established, and set a target for standard effluent quality to preserve water quality, and protect the aquatic ecosystem; wastewater needs to be treated before discharge to receiving waters to satisfy these standard regulations.

## 2.2 Conventional Wastewater Treatment Process

### 2.2.1 Overview of Wastewater Treatment Process

Wastewater treatment was first developed to prevent negative impacts on the environment and public health. As the population increased significantly, the amount of wastewater generated rose rapidly and exceeded the self-purifying capacity of receiving water bodies. From 1900 to the early 1970s, the main aim of wastewater treatment was to remove suspended and floatable material, BOD and disease-causing pathogenic bacteria [17]. Wastewater treatment was later focused primarily on aesthetics and environment from the early 1970 to 1990s [32], however, the existing requirement remained valid but at higher levels. Nutrient removal started to be addressed in some streams, and as a consequence, this increased understanding of the environmental effect caused by wastewater, and knowledge of negative impacts caused by the specific components in wastewater [33]. Wastewater treatment has also focused on the heath concerns regarding toxic and potential toxic chemicals discharged into the environment since 1990 [34]. While the earlier treatment objectives remain valid, the degree of treatment and treatment objectives have increased significantly; this can be achieved through appropriate wastewater treatment processes [17, 34].

Sewage/wastewater is necessarily treated before discharge into the environment. To treat wastewater, organic matter and other pollutants are removed from wastewater to an acceptable level before discharge. Based on wastewater regulations this does not require specific technologies, so the systems for collecting, treating and disposing municipal wastewater vary widely in terms of processes used and equipment. In order to satisfy the level of contaminant removal which is typically enforced by local regulations, biological, chemical and physical processes are used to remove contaminants from the wastewater, and these methods are combined into various linked systems, classified as preliminary, primary, secondary and tertiary treatment [7, 35] (Figure 2.1) as follows.

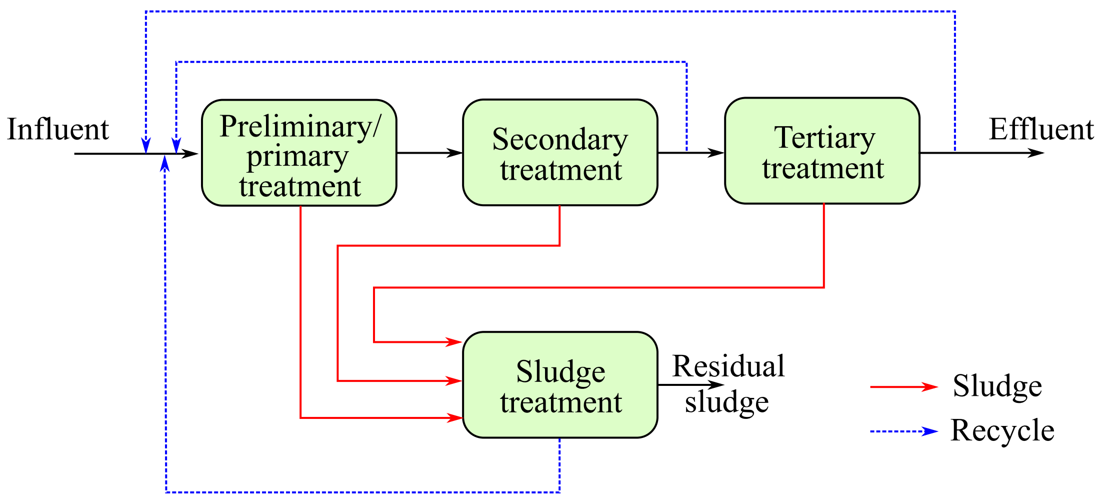



Figure 2.1: Levels of wastewater treatment processes.

#### 2.2.1.1 Preliminary Wastewater Treatment

Preliminary wastewater treatment involves the removal of wastewater constituents which may cause maintenance or operational problems in subsequent processes. It solely separates the floating materials (tree branches, papers, pieces of rags, wood etc) and the heavy inorganic solids. Examples of prelimanary unit operations include screening (removal of debris and rags), grit removal (removal of coarse suspended matter) and floatation (removal of oil and grease).

#### 2.2.1.2 Primary Wastewater Treatment

A portion of the organic matter and suspended solids are removed in primary treatment. The liquid effluent from primary treatment may still have a high BOD (around 60% of wastewater influent), and contain large amounts of suspended organic matter. The separated organic solids from this stage are sometimes stabilized by anaerobic digestion, or incinerated for energy recovery; the remains from sludge stabilisation is used either for landfill or fertilizer. The removal is achieved by sedimentation and some chemicals such as metal salt and polymers as organic polyelectrolytes [36] may be added to enhance solids removal.

#### 2.2.1.3 Secondary Wastewater Treatment

After primary treatment, wastewater is sent to secondary treatment to remove organic matter and any remaining suspended solids by means of biological treatment, either under aerobic or anaerobic conditions. In biological treatment, biomass decomposes the organic matter to produce a clearer effluent, and the effluent from secondary treatment usually contains very little BOD (5-10% of wastewater influent), and small amounts of DO. Biosolids or sludge separated in the secondary settling tanks is sometimes disposed by stabilizing it under anaerobic conditions (similar to the primary sludge). Aerobic treatment is commonly used as secondary wastewater treatment, e.g. the activated sludge process, because it is the most conventional approach to removing organic matter and nutrients, and is very flexible in achieving specific effluent requirements, although it needs a large amount of energy, mostly for aeration to maintain an aerobic population of bacteria in the bioreactor. Anaerobic treatment, on the other hand, requires less energy consumption and some portion of the potential energy can be recovered. Due to the energy crisis in the 1970s, research attention has been shifted from aerobic to anaerobic wastewater treatment [33]. However, bacteria under the anaerobic condition require longer retention times due to their slow growth, and it has a very little effect on nutrient removal.

#### 2.2.1.4 Tertiary/Advanced Wastewater Treatment

Tertiary treatment involves additional treatment beyond the secondary treatment or the final cleaning process to improve wastewater quality before being reused, recycled or discharged to the environment. The majority of BOD and suspended solids found in wastewater are removed in the primary and secondary stages. This stage of treatment is particular important in the sensitive or fragile ecosystems, e.g. estuaries, coral reefs and rivers to protect those areas and/or to meet requirement standards of directives. The tertiary treatment would be tailored to specific contaminants [37]. This includes filtration, disinfection and nutrient removal. It is also known as "advanced treatment" where nutrient removal is included. The following section provides further details about nutrient removal in wastewater treatment.

### 2.2.2 Nutrient Removal

Nutrients, especially nitrogen and phosphorus are of considerable concern in wastewater discharge. Discharging these nutrients into receiving waters may stimulate the growth of algae/rooted aquatic plants in shallow streams, and lead to eutrophication. Large amounts of nitrogen and phosphorus can also have other negative effects such as: toxicity to aquatic life ($NH_3$), chlorine disinfection efficiency ($NH_3$ to chloramines), depletion of dissolved oxygen due to nitrogenous oxygen demand (oxidation of ammonia to nitrate), and creation of a public health hazard (e.g. infant methaemoglobinaemia from nitrate ingestion [38]). Phosphorus and nitrogen can be removed by either biological, chemical or physical methods, as described below.

#### 2.2.2.1 Nitrogen Removal

Nitrogen is an important nutrient for the growth of biological life, and one of the primary components in living organisms. However, excessive amounts of nitrogen in wastewater can be toxic for aquatic organisms, eg. fish, and cause eutrophication. Nitrogen in wastewater can be present in several forms, e.g. ammonia, nitrate, nitrite and organic compounds; most nitrogen in wastewater is in the form of ammonium and ions that are difficult to remove. Typically, nitrogen is removed through biological processes consisting of two steps, nitrification and denitrification, and each step requires different environmental conditions. Complete nitrification is performed through two sequential oxidative steps by autotrophic bacteria under aerobic conditions. Each step is carried out by different bacteria genera which use ammonia or nitrite as an energy source, and oxygen as an electron acceptor, while the carbon source used is carbon dioxide. In the first step, ammonia is oxidized to nitrite by a group of autotrophic bacteria called Nitroso-bacteria or Ammonia Oxydizing Bacteria (AOB), and *Nitrosomonas* is the most commonly recognized genus of bacteria to perform ammonia oxidation (2.1) [39]:

$$\mathrm{NH_4^+} + \frac{3}{2}\mathrm{O_2} \longrightarrow \mathrm{NO_2^-} + 2\mathrm{H^+} + \mathrm{H_2O} \tag{2.1}$$

Then nitrite, which is a product of ammonia oxidation, is further transformed into nitrate by another group of autotrophic bacteria called Nitro-bacteria or Nitrite Oxidizer Bacteria (NOB). *Nitrobacter* is the most commonly recognized nitrite oxidizer [39]:

$$\mathrm{NO_2^-} + \frac{1}{2}\mathrm{O_2} \longrightarrow \mathrm{NO_3^-} \tag{2.2}$$

Autotrophic nitrifying bacteria are more sentitive to environmental conditions, and their growth rate is relatively slower than heterotrophic bacteria [39]. As a result, the retention time required for biomass in nitrifying reactors is necessarily longer than treatment systems for COD removal in order to have enough time to grow the nitrifying bacteria. The growth rate of nitrite oxidizing bacteria depends on ammonia oxidizing bacteria for their nitrite supply, although it is higher.

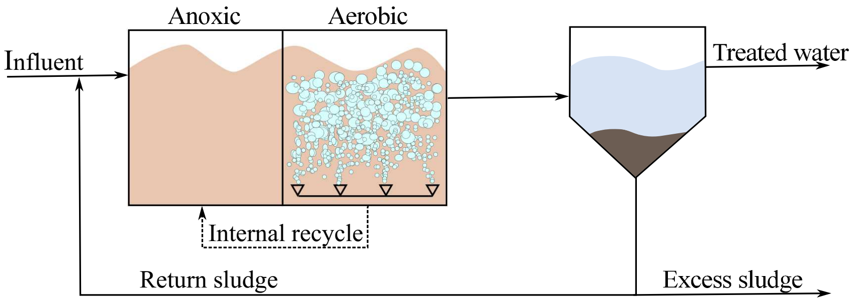
Denitrification involves nitrate reduction, thereby transforming it to nitrogen gas, and is carried out by facultative heterotrophic or autotrophic bacteria under anoxic conditions. For the heterotrophic denitrifers, biological denitrification is the oxidation of organic substrates in wastewater which use nitrate or nitrite as the electron acceptor. Nitrate reduction involves several steps from nitrate to nitrite, nitric oxide, nitrous oxide, and finally nitrogen gas. If the process is not complete, nitric oxide (NO) and nitrous oxide ($N_2O$) can be emitted, which can contribute to smog and GHGs, respectively.

$$6NO_3^- + 5CH_3OH \longrightarrow 5CO_2 + 3N_2 + 7H_2O + 6OH^- \tag{2.3}$$

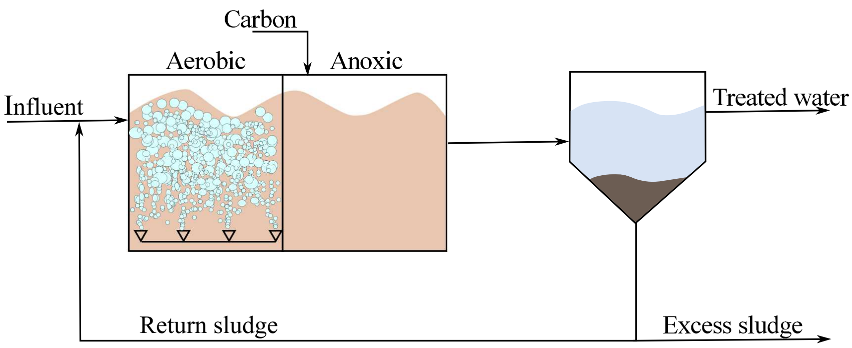
For autotrophic bacteria, inorganic compounds, e.g. sulphur, iron and hydrogen are used as electron donors instead of organic carbon for growth, and nitrate is still used as an electron acceptor, while organic carbon is obtained from carbon dioxide. The main advantage of autotrophs over heterotrophs is that it is easier to manage and maintain inorganic compounds than organic carbon [40].

Nutrient removal can be achieved through severa options in wastewater treatment processes, e.g. activated sludge, trickling filters, membrane bioreactor (MBR), moving bed biofilm reactor (MBBR). However, activated sludge is commonly used for organic and nitrogen treatment for both domestic and industrial wastewater because it has been proven successful and reliable [41, 42]. The simplest activated sludge system consists of two main components: the bioreactor or the aeration tank and clarifier. Biomass or bacteria in the bioreactor convert soluble and colloidal biodegradable organic matter, nutrients and certain inorganic compounds into cell mass and metabolic end products. Then, treated water and biomass are separated in the clarifier by means of sedimentation. The activated sludge system was developed by Arden and Lockett in 1914 [43], and has becoming very popular all over the world. Activated sludge has also been applied for nitrification and denitrification by changing its environmental conditions; for instance, high levels of oxygen are supplied for nitrification under aerobic conditions, although isolated anoxic and aerobic reactors are usually used (pre-denitrification and post denitrification). There are typically three main process configurations for biological nitrogen removal (BNR), and for the preanoxic denitrification (Figure 2.2a), which is a sequence of anoxic and aerobic tanks. The nitrate produced in the aerobic zone is recycled back to the anoxic zone to combine with the carbon source available in the influent for denitrification to occur. The postanoxic configuration (Figure 2.2b), on the other hand, is the sequence of the aerobic and anoxic zones. This approach requires the external carbon source added in the anoxic zone to perform denitrification because most of the organic carbon available for denitrification in the wastewater influent may be already degraded in the aerobic zones. In the third configuration, nitrification and denitrification occurs in one bioreactor, and an alternating operational strategy is carried out between aeration and no aeration periods. The aeration period when COD oxidation and nitrification are performed alternates with a period of no aeration when the biomass depletes the oxygen to create anoxic conditions for denitrification.

However, conventional nitrogen removal based on nitrification and denitrification is an energy intensive process. Over the last few decades several new and cost-effective nitrogen removal processes have been developed. Anaerobic ammonium oxidation (Anammox process) is a promising technology among a variety of alternatives, and may be suitable for the treatment of nitrogen-rich wastewater. The discovery of Anammox bacteria provides a better understanding of the nitrogen cycle, and was first discovered in a denitrifying fluidized bed reactor [44]; ammonium is oxidized to nitrogen gas by autotrophic Anammox bacteria under anoxic condtions. Anammox has advantages in terms of smaller reactors, higher nitrogen removal rate, and lower operational costs. It has been successfully implemented at the laboratory, pilot and full scale to treat ammonium-rich wastewater, e.g. supernatants from anaerobic digestion [45]. However, ammonium is required to be partly preoxidized to nitrite before the Anammox process, and as a result Anammox needs to be operated in sequence with a partial nitrification process such as a single reactor high activity ammonium removal over nitrite process (SHARON®) [46]. SHARON® was developed for ammonia removal through the nitrite route, and provides appropriate influent conditions for the Anammox reaction. The partial nitrification is typically performed in a single stirred tank with suitable conditions (no sludge retention, about 1 day HRT, 30-40 °C and 6.6-7 pH) and this results in a stable nitrification with nitrite [47].




(a)




(b)

Figure 2.2: Activated sludge with nitrification and denitrification processes; a) preanoxic, b) postanoxic.

#### 2.2.2.2 Phosphorus Removal

Phosphorus removal can be achieved using either a chemical or biological process, or a combination of both. The chemical precipitation of phosphorus was used in Paris in 1740 with lime [48] and with alum/iron salts [49]; the method is relatively simple and well established in several countries around the world. It involves the addition of metal salts to wastewater resulting in the precipitation of an insoluble metal phosphate which is separated by sedimentation; metals such as calcium, iron and aluminium are normally added, while lime and anionic polymers may also be used to precipitate and assist solids separation. Chemical precipitation for phosphorus removal is very flexible and can be implemented at several stages during wastewater treatment. In addition, chemical precipitation produces phosphorus bound up as a metal salt in the waste sludge, which could provide potential value when it is used in agriculture. However, this approach results in high reactive chemical costs, and produces additional sludge. Several studies have attempted to develop alternative technologies that can offer more value and a consistent product for recycling phosphorus to other applications [50].

Biological phosphorus removal is more complicated involving a group of bacteria called PAOs (Phosphorus Accumulating Organisms), and is based on switching the system between anerobic and aerobic conditions. During anaerobic conditions PAOs store organic compounds such as VFAs as PHA (Polyhydroxyalkanoates) which are then degraded for growth and respiration. At the same time, phosphate is assimilated into cells and the storage of polyphosphate is increased. Phosphorus removal occurs when sludge with the accumulated phosphorus is removed, as illustrated in Figure 2.3. Biological phosphorus

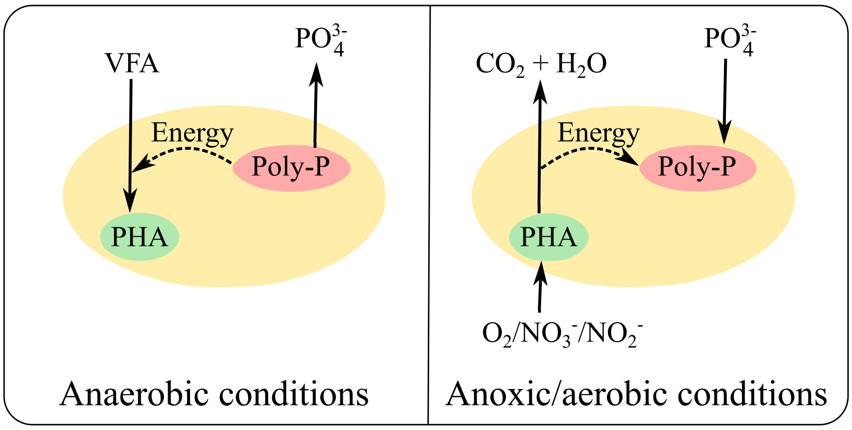



Figure 2.3: Mechanism of biological phosphorus removal modified from Ostace [51].

removal is commonly achieved in the activated sludge process, thereby placing an anaerobic and/or anoxic zone ahead of an aerobic zone. In the anaerobic zone where oxygen and nitrate is not available, bacteria take up the VFAs and release phosphorus in the form of phosphate into solution. Then bacteria in the aerobic zone can uptake phosphorus, which increases overall phosphorus removal to as much as 80-90%. Over the past several decades, biological treatment systems for simultaneous nitrogen and phosphorus removal have been developed and the anaerobic-anoxic-aerobic (A2O) process (Figure 2.4) is the most simple, common and practical process [52]. However, efficiency of biological phosphorus removal is generally low, and it requires chemical precipitation in order to result in high and consistent removal.

Over the years, sewage sludge has been used in agriculture because it contains useful nutrients, e.g. phosphorus and nitrogen. Phosphorus is an important, yet limited resource that cannot be replaced by other elements, and is one of the main nutrients for plant growth. With increasing populations, the demand for food crops and hence phosphorus consumption has grown significantly. However, the supply of phosphate rock is expected to be depleted in the near future [53], and a number of researchers have attempted to recycle phosphorus in wastewater [54, 55]. Currently, phosphorus recovery is attracting considerable attention, and there have been various approaches developed which will be discussed in the section on resouce recovery.

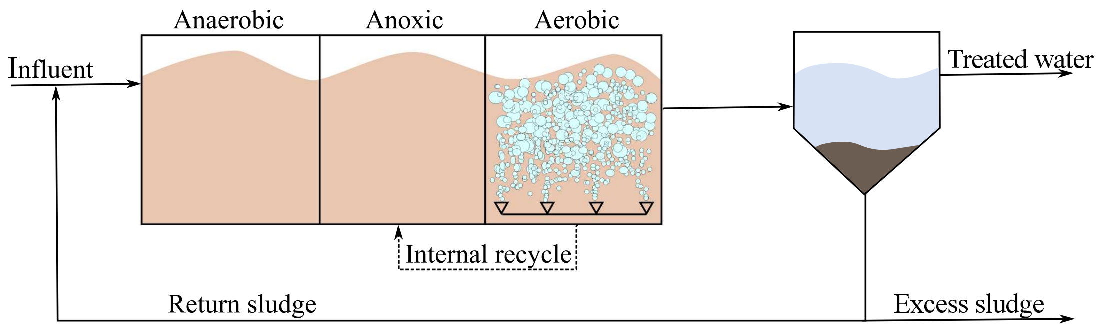



Figure 2.4: Biological phosphorus removal (A2O) process.

### 2.2.3 Biosolids Treatment

Biosolids or sludge treatment is a critical issue because a large amount of sludge is produced as a waste or by-product from conventional WWTPs, and it is one of the most challenging economic and environmental problems in wastewater treatment [56, 57]. Typically, sludge from wastewater treatment processes is in liquid form, and its characteristics are dependent on influent composition and the treatment units used. Solids in wastewater influents are usually removed in the primary clarifier, while organic solids are generated and removed in the secondary treatment or thickening process. The main aim of sludge treatment is to reduce the sludge volume to reduce handling and transport costs, to prevent odour, and to eliminate disease-causing bacteria. Sludge treatment firstly needs to reduce the water content of raw sludge, and to transform complex organic matter into a relatively stable and inert residue. The residue from sludge treatment is required to meet conditions for disposal acceptance regulations, and several alternatives for sludge disposal include agricultural reuse, incineration, gasification etc.

Sludge treatment for municipal WWTPs typically consists of the processing steps, as shown in Figure 2.5. A first step is to thicken the sludge by means of gravity, flotation

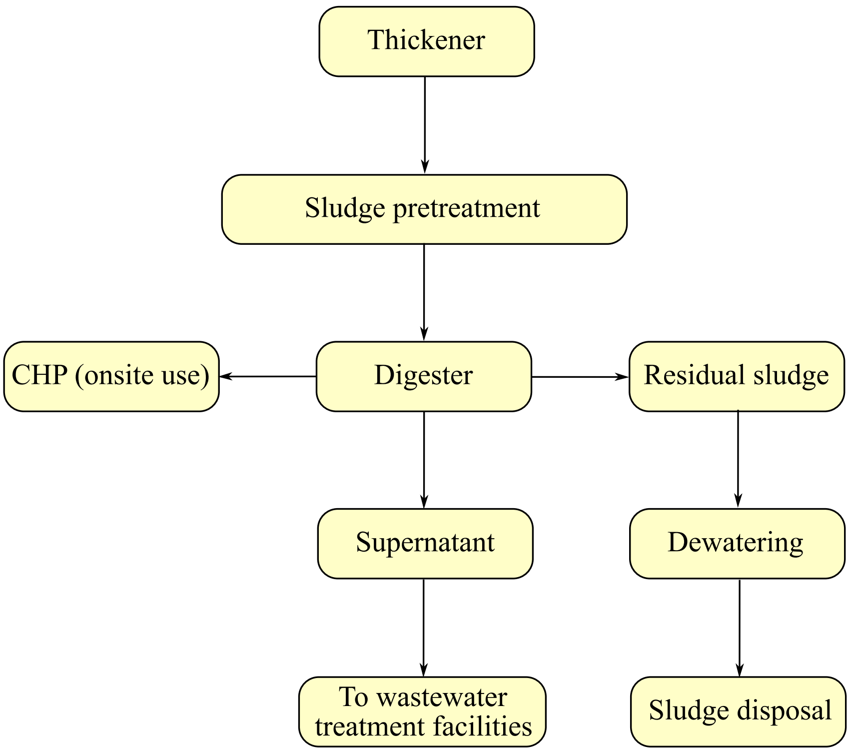



Figure 2.5: Schematic representation of sludge treatment modified from Appels et al. [58].

or filtration. The separated water or supernatant is sent back to the head of the WWTP, and the thickened sludge is subjected to some form of stabilization. Anaerobic digestion is the most widely used technique for sludge stabilization, and has been for over 100 years, but is now receiving enhanced attention because of its ability to transform organic matter into biogas (70% methane), and reduce the amount of sludge for disposal; it also considerably reduces the pathogens in sludge. Anaerobic digestion involves the biological oxidation of organic matter without oxygen to produce end-products such as methane and carbon dioxide. It is used for stabilizing the sludge, reducing the overall load on sludge disposal [58], enhancing sludge dewatering ability and reducing microorganisms. It also converts part of the organic matter into biogas which is used as an energy source to reduce operating costs, and the amount of biogas produced from anaerobic digestion depends on the sludge composition [59]. Anaerobic digestion of organic matter basically consists of four stages: hydrolysis, acidogenesis, acetogenesis and methanogenesis, as illustrated in Figure 2.6. In the first stage, insoluble organic material and complex organic matter such

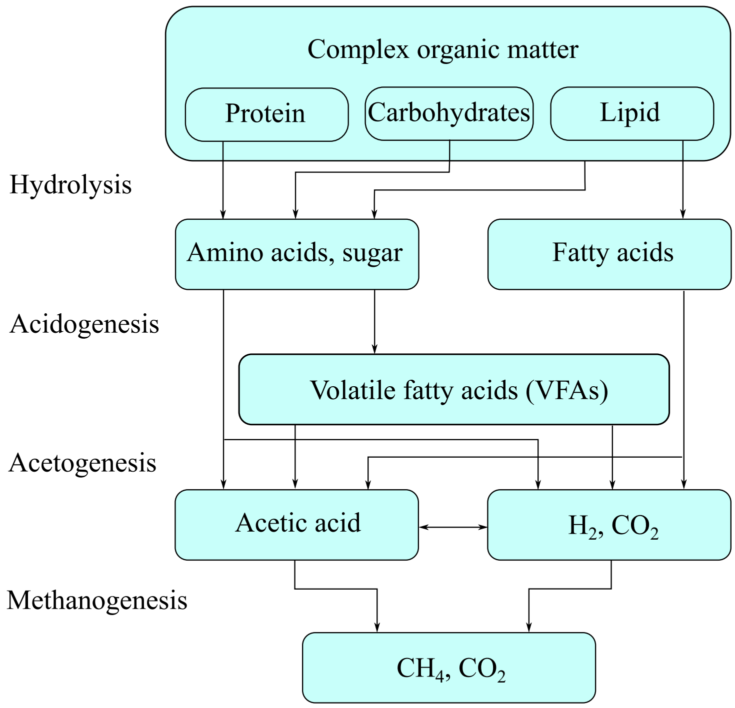



Figure 2.6: Subsequent stages in the anaerobic digestion process of organic matter.

as carbohydrates, protein, lipids are hydrolyzed into smaller soluble organic substances, e.g. amino acids, sugar and fatty acids, and hydrolysis is often the rate-limiting stage in anaerobic digestion. These substances from hydrolysis are further degraded in the second stage, where volatile fatty acids (VFAs) along with ammonia, $CO_2$, $H_2S$ and other by-products are produced by acidogenic bacteria. Later, the VFAs are degraded in the acetogenesis stage to produce acetic acid, $CO_2$ and $H_2$, and the partial pressure of $H_2$ controls this conversion. Finally, methane is produced by two groups of methanogenic bacteria in the methanogenesis stage. In the first group, acetic acid is split into methane and $CO_2$, whereas in the second group $H_2$ as the electron donor combines with $CO_2$ as an electron acceptor to form methane. The digested sludge has a tar-like consistency, and smells ammoniacal. Anaerobic digestion also conserves nutrients, which are more available to plants and reduce the quantity of sludge produced, and is practically combined with a combined heat and power generation (CHP) unit to produce renewable energy in the form of electricity and hot water. However, the requirement for long retention times and high temperatures ( 35 °C) are drawbacks for this treatment due to the slow growth rate of methanogenic bacteria. Several studies have focused on increasing the amount of sludge, improving mixing in digesters and increasing biogas yield (increasing solids destruction). For example, conventional anaerobic digesters require large residence time and large volumes due to the slow degradation rate of anaerobic digestion and sludge hydrolysis is the rate-limiting step. The use of ultrasound, microwaves, high pressure homogenizers, enzymatic and themal hydrolysis break open cells to increase solids destruction, stability at the shorter residence time and biogas production [60, 61] because degradability is improved. These techniques also improve the subsequent process e.g. dewatering and sanitisation of sludge and the odour.

Residue sludge after stabilization is transferred to the dewatering unit to further reduce the sludge volume. Dewatered sludge contains 20-35% dry solid (65-80% moisture), and depends on the type of sludge and its dewatering. A conditioner is typically added to flocculate the particles, and free water is removed. Dewatering is an important step before utilizing sludge in subsequent processes. For example, the cost of thermal drying is directly related to the effectiveness of dewatering because it has an effect on the amount of water to be evaporated. It is interesting to note that the better the dewatering, the better and easier the sludge would be to be used in subsequent processes. Supernatant from the dewatering unit is normally returned to the inlet of the wastewater treatment process because it contains high levels of nitrogen, phosphorus as well as being warm. The return supernatant can make the process more efficient as there are a number of treatment methods which are not commonly used with the main wastewater stream, such as Anammox and nutrient recovery.

## 2.3 Energy Use in WWTPs and GHGs Emissions

Wastewater treatment is an energy intensive process as all steps in wastewater treatment require energy for mixing, pumping and aeration. Energy consumption in WWTPs depends on the location of the plant, size (population, organic/hydraulic loading), wastewater characteristics and effluent requirements. The specific power consumption can be attributed to the difference in the scale of the plants rather than different kinds of WWTPs [62]. Typically, electricity consumption for wastewater treatment is about 1% (7,703 GWh/year) of the total UK demand, making it the fourth most energy intensive sector [63] in the UK economy. WWTPs require energy in the range of 0.5-2.0 kWh/m$^3$, but less than 0.5 kWh/m$^3$ for wastewater treatment without nutrient removal [64]. Different stages in conventional WWTPs require different energy uses. Bodík and Kubaská [65] reported on the specific energy demands of three treatment stages, which vary widely in different countries, as presented in Table 2.1.

- **Preliminary/Primary treatment** - This includes wastewater collection, pumping, screening, grit removal and sedimentation in the primary settling tanks. The processes in this treatment step requires relatively low energy use (except wastewater pumping). The average or range of energy consumption varies widely in the literature from different countries. Sludge pumping is generally considered as the largest energy use. However, efficiency of primary treatment affects energy use in secondary treatment; for example, a lower efficiency in primary treatment may require more energy in terms of aeration to remove organic matter and nutrients in secondary treatment.

- **Secondary treatment** - Aeration is considered to require the largest amount of energy in secondary treatment. Typically, the aeration energy in biological treatment with nutrient removal can represent up to 50% of the overall WWTP operating costs, or even higher [64]. Along with aeration, mixing and recirculation require significant energy use, especially in the activated sludge system. Similarly, the range of energy use in secondary wastewater treatment varies widely from country to country [65].

- **Tertiary treatment** - This stage requires a relatively large amount of energy because of the demands from nutrient removal processes such as nitrification, denitrification and biological P removal. Additionally, energy use can be even larger for water reclamation/reuse, which may require advance treatment technologies such as reverse osmosis to purify wastewater. It is worth noting that this treatment stage is defined differently between countries.

Table 2.1: Energy use of primary, secondary and tertiary treatment in different countries [65].

| Country | Energy consumption, kWh/m$^3$ |
|---|---|
| **Primary treatment** | |
| USA | 0.04 |
| New Zealand | 0.04 -0.19 |
| Canada | 0.02 - 0.1 |
| Australia | 0.01 - 0.37 |
| **Secondary treatment** | |
| Australia | 0.305 |
| China | 0.29 |
| Japan | 0.304 |
| USA | 0.2 |
| Sweden | 0.42 |
| **Tertiary treatment** | |
| Japan | 0.39-3.74 |
| USA | 0.43 |
| Taiwan | 0.41 |
| New Zealand | 0.49 |
| Hungary | 0.45-0.75 |
| Singapore | 0.72-0.92 |

More specifically, a domestic WWTP with activated sludge and anaerobic sludge digestion consumes around 0.6 kWh/m$^3$ of treated wastewater, which results mainly from the supply of air for the activated sludge. However, biogas produced from sludge treatment through anaerobic digestion can reduce the energy use for activated sludge by 25-50%. It is worth noting that further plant modifications may be able to reduce energy consumption substantially, and capturing more energy can potentially transform wastewater into a net energy producer instead of consumer [66]. Other wastewater treatment processes including lagoons, trickling filters, activated sludge and advanced wastewater treatment use energy of 0.09-0.29, 0.18-0.42, 0.33-0.6 and 0.31-0.4 kWh per $m^3$ treated wastewater, respectively [64]. Figure 2.7 represents typical energy use in a 10 million gallons per day

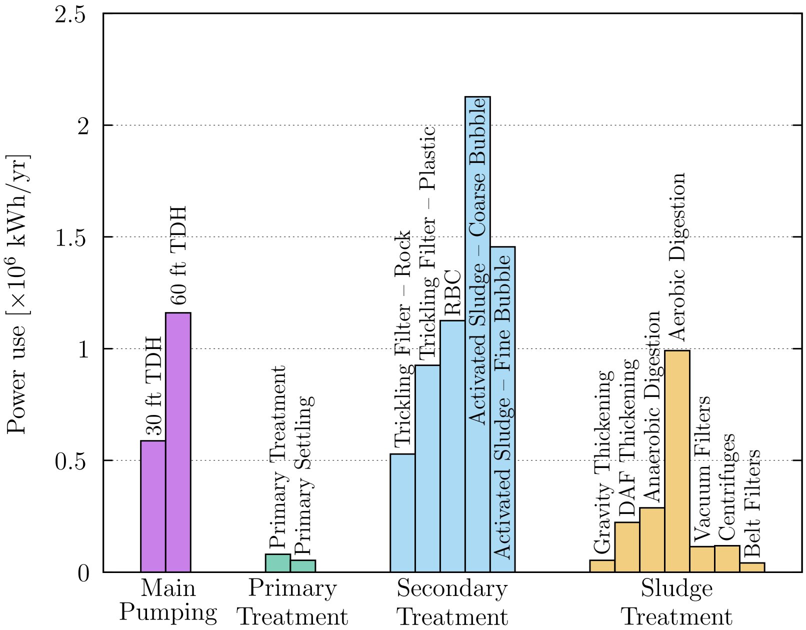



Figure 2.7: Typical energy use profile for 10 MGD WWTPs, modified from Owen [67].

(MGD) conventional WWTP with commonly used unit operations and processes. However, the energy consumption of WWTPs with smaller hydraulic capacities and more advanced treatment technologies generally require larger amounts of energy per unit volume.

Together with energy consumption, the WWTP is a source of greenhouse gas (GHGs) emissions which are responsible for global climate change. It is found that around 45 million tons of $CO_2$ is emitted annually in the U.S. because of organic waste degradation apart from the GHG emissions generated from energy consumption [64]. Additionally, worldwide wastewater is the fifth largest source of fugitive anthropogenic methane ($CH_4$) emissions. Worldwide wastewater contributes to 3% of the total nitrous oxide ($N_2O$) emissions, which is the sixth largest emission source [68]. Tribe [69] studied carbon emissions from WWTPs at different levels of ammonia discharge based on tertiary nitrifying trickling filters. The specific carbon emissions were around 2.2 $tCO_2e/tNH_3$-N removed for the ammonia discharge of 5 mg/L through nitrification. The situation was even worse because the specific carbon emission rises significantly by almost 50% for an ammonia discharge of 1 mg/L, as illustrated in Figure 2.8. Quantitatively, the whole life carbon emissions over 40 years of a WWTP with 200,000 population equivalents is around 455,908 $tCO_2e$ (11,398 $tCO_2$/yr). It was found that the carbon emissions were dominated by carbon from indirect emissions due to electricity use from the grid, and onsite generation. In addition,

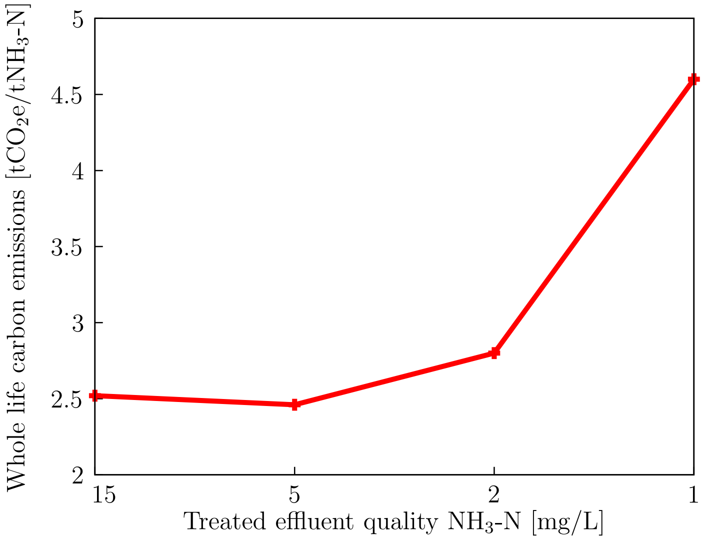



Figure 2.8: Whole life carbon and effluent quality for tertiary WWTPs, modified from Tribe [69].

the biological approach for nitrogen removal based on nitrification and denitrification can contribute to the generation of nitrous oxide ($N_2O$). This is of particular concern because the radiative forcing of $N_2O$ is 300-fold stronger than $CO_2$, and it can react with ozone in the stratosphere which can result in ozone layer depletion. Thus, small amounts of $N_2O$ can potentially have an adverse impact on the environment. Ni et al. [70] reported that $N_2O$ emissions currently accounts for 0.1-25% of the consumed nitrogen in the nitrification and denitrification processes.

### Interaction inside Wastewater Treatment Processes

After considering various wastewater and sludge treatment processes in WWTPs, it is also important to view the whole picture of processes and interactions amongst them. This is because it has effects in several aspects in terms of process operation, effluent quality, energy use and environmental impacts. Although it is more convenient to consider one unit at a time, this may loose sight of interactions amongst them, and the interaction between various treatment/ separation units makes process design and operation more difficult to handle. Treated wastewater from one unit will affect the subsequent units, and recycling within the plant makes the overall operation more complex. Similarly, the total energy consumption and fugitive emissions in WWTPs are a function of interactions among the treatment/ separation units. For instance, energy use for secondary treatment is a function of primary treatment performance, and likewise, the energy requirement for sludge treatment is affected by both primary and secondary treatment. Most stabilisation processes are energy efficient when organic matter is concentrated before treatment, and depending on the wastewater characteristics, primary treatment can remove and concentrate organic matter by means of physical separation using small amounts of energy. However, organic matter is not stabilised in this process and thus subsequent stabilisation processes are required. In many applications, the energy cost for removing and concentrating organic matter in primary treatment can save a large amount of energy that is otherwise required for subsequent processes. For example, the wastewater influent is split in primary treatment: a fraction of solids is conveyed to sludge treatment, while the remainder is sent to secondary treatment. Organic matter can be treated either in the secondary treatment process or in sludge treatment (which includes secondary waste activated sludge). If energy efficiency in sludge treatment is higher than in secondary treatment, the preferred method is to remove as much organic matter as possible in the primary treatment, sending this organic load to sludge treatment. In the case where there is no primary treatment and the total organic matter is conveyed to secondary treatment, this can lead to an increase in energy consumption [67].

Design and operation of secondary treatment will determine the fractions stabilised in each sequence. In activated sludge, for example, SRT is used to determine the degree of stabilisation, and this is more complete at long SRTs (less waste sludge generated).

However, energy consumption due to aeration is higher at longer SRT. Sludge treatment, e.g. anaerobic digestion, is also affected by activated sludge from waste sludge production. When considering nitrification at long SRTs, the effect of secondary treatment SRT on energy consumption can be more dramatic, but in general, shorter SRTs lead to overall system energy efficiency. However, if sludge treatment is not energy efficient, the converse of the above situation holds true. For medium and large scale WWTPs, wastewater influent typically undergoes primary settling to remove 50-70% of the particulate matter [17]. Primary settling has effects on both wastewater and sludge treatment, which turns out to be lower oxygen demand and higher energy recovery. A practical approach to enhancing primary sedimentation can be through chemical precipitation by adding metal salts and/or polymers to enhance precipitation. The addition of chemicals can cause the suspended particulates to aggregate together through coagulation and flocculation. However, this may decrease the efficiency of nutrient removal in terms of denitrification due to the absence of a carbon source. Gori et al. [71] investigated the effect of primary sedimentation on the energy footprint of wastewater treatment processes. Primary sedimentation increases the solid fraction of COD sent to anaerobic digestion, and this leads to an increase in biogas production, and energy recovery of up to 130%. It could also reduce energy consumption by up to 13.5% compared to a scenario without primary sedimentation.

## 2.4 Sustainable WWTPs

Economic and environmental crises have steadily increased due to an increase in energy use and GHGs emissions, and the foreseeable depletion of non-renewable resources. These problems have driven WWTPs toward a more sustainable utilization of wastewater, however, solving such problems is not a straightforward task. Baleta and McDonnell [72] pointed out that there are conflicts between the European Union Water Framework Directive (EU WFD) and the United Kingdom Climate Change Act (UK CCA). The EU WFD aims to achieve good ecological and chemical status in inland and coastal waters by

2015, which can be implemented by increasing effluent quality standards and removing hazardous components from wastewater discharge. However, this requires addtional treatment and consequently more carbon emissions, and it is estimated by the WFD that this will result in an increase of 110,000 tonnes of carbon emissions per year.Unfortunately, this contradicts the UK CCA policy which aims to reduce GHG emissions by 80% by 2050 from the baseline levels in 1990. Additionally, problems regarding climate variability, e.g. rising temperature, drier summer, and more intense rainfall, can lead to a worsening of the situation, e.g. risks of higher water demand from drought or flooding. Such contradictions with respect to carbon emissions reduction and effluent quality requirements present a moral dilemma in comparing two conflicting situations.

Sustainability as defined in Chapter 1 is becoming an increasingly important criterion in WWTPs, but current practices in WWTPs are typically energy intensive and require large investments, as well as operating costs. In addition, there is a significant amount of both offsite and onsite GHGs emissions such as $CO_2$, $CH_4$, $N_2O$ and other volatile compounds. At the same time, excess sludge is being produced and needs further treatment and disposal. Finally, most of the valuable resources in wastewater such as $NH_4^+$-N, $PO_4^{3-}$-P and heavy metals are removed instead of being recovered; without improvement and process modification these can lower process sustainability significantly. Recently, effort has been made by the wastewater treatment community to improve sustainability, which includes the optimisation of energy use, resource recovery, efficiency of equipment and energy costs.

For instance, the Strass WWTP in Austria has undergone excellent improvements towards being more sustainable. It serves approximately 60,000-250,000 population-equivalent, depending on the season (peak during the tourist season in the winter) and consists of a two-stage biological treatment to remove organics and nutrients. Several efforts were made to produce more electrical energy than the energy required for its operation. These include a reduction in chemical cost and energy consumption through replacing old equipment with new/more efficient equipment, changing control/operational strategies and implementing a sidestream nitrogen removal (DEMON®). Additionally, new co-generation was used to enhance the efficiency of electricity production. The WWTP could produce energy of up to 8,500 kWh/day, while requiring only 7,869 kWh/day [73], and hence was energy neutral. It becomes clear that WWTPs have considerable potential to become a sustainable process, or even an energy exporting one. More generally, two main approaches may be used in WWTP in order to improve sustainability, namely energy efficiency and resource recovery.

### 2.4.1 Energy Efficiency for WWTPs

Water quality is the main concern in the wastewater industry to keep public trust [74]. WWTPs are traditionally designed to meet effluent requirements without taking energy efficiency into account. Their design and operation are mostly based on intuition and experience [17], rather than on optimal conditions [75], and hence WWTPs consequently use a large amount of energy for process operation. More specifically, energy distribution in a conventional WWTP is shown in Figure 2.9. It can be clearly seen that aeration accounts for significant energy use, ranging from 50-75% of the total energy consumption [64]; wastewater pumping and anaerobic digestion are also major energy intensive processes. Recently, energy efficiency has played an important role in achieving sustainability, and there is even more potential to slow the increase in energy use through improving energy efficiency while improving wastewater treatment. It is obvious that higher energy efficiency can offer lower energy use, GHGs emisssions and operating costs for WWTPs [76]. Energy efficiency can be achieved through several approaches, including control and operational changes, and replacing and retrofiting inefficient equipment. Energy use in WWTPs can be reduced significantly by replacing and/or retrofitting existing equipment, e.g. pumps with better-sized and higher efficiency equipment. Practically, equipment should be evaluated regularly in terms of its condition, performance and remaining lifetime. Aging equipment which has reached the end of its lifetime, is typically inefficient

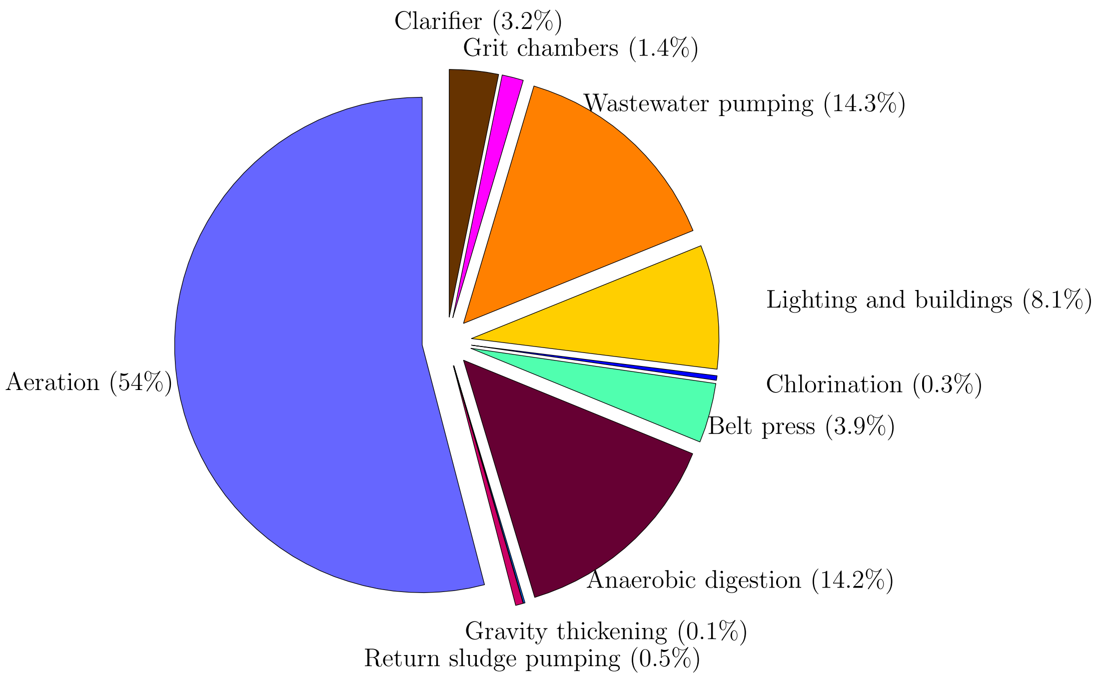



Figure 2.9: Distribution of energy requirement for conventional WWTPs in U.S., modified from Gude [64].

and requires more energy than new equipment. While this concept requires capital investment for purchasing new equipment, energy saving costs could be more effective over the life cycle. Several assumptions were probably made in the conservative design of previous equipment, including the use of design guidelines, engineering experiences, safety factors and a worst case scenario, which may lead to an oversized design. Consequently, the operation may be far away from its optimal conditions, and the replacement of the old pumps with higher effciency pumps or a new model can typically save around 5-15% of its energy costs [77]. For instance, the East Bay Municipal Utility District (EBMUD) in northern California treats 1.57 billion litres of wastewater a day. Several energy efficiency measures were implemented, which included replacing two smaller compressors with one large unit, and installing a higher efficiency motor with variable frequency drives (VFDs). This led to a reduction in electricity use by the pumps of around 50% [78].

Energy efficiency can be implemented through a modification of control and operational strategies. It is important to understand how the individual treatment/separation units in WWTPs are operated, and how they affect the other units, because setpoints of some units, e.g. DO level can be changed within the design limits. Better control and operational strategies can offer opportunities to reduce energy use and GHGs emissions while still maintaining effluent quality within the regulatory limits. However, control and operational strategies for WWTPs are different from plant to plant, and may vary by time of day, season, and/or other characteristics. Evaluating influent and effluent trends regularly can help improve control and operational strategies. Improving control and operational strategies in WWTPs such as adjustment of the aeration capacity and flowrate involves a reduction in energy use, and can typically save more energy than equipment upgrades without any capital investment requirements [79]. It is interesting to note that the aim of this approach is to achieve an optimal balance between effluent quality and energy. Several attempts in the wastewater treatment community have been made to optimise aeration through controlling a dissolved oxygen setpoint due to the fact that aeration is an energy-intensive process. Åmand et al. [80] investigated an approach to control aeration to reduce energy consumption while satisfying effluent discharge standards. The results show that the air flow requirement can be reduced around 1-4% in comparison with the constant dissolved oxygen set point, and 14% in comparison with fast feedback of effluent ammonium, thereby changing the control and operational strategies. Recently, Mamais et al. [81] assessed energy consumption and GHG emissions in Greek WWTPs ranging from 10,000 to 4,000,000 population-equivalents (PE), and used a mathematical model to evaluate the proposed energy saving strategies through changing control/operation strategies. The results of this case study show that there is a potential to reduce both energy use and GHG emissions by up to 4.5 MWh/yr, through the reduction of dissolved oxygen set points and sludge retention times.

Although WWTPs consume a large amount of energy, it is possible to recover/generate renewable energy within the plant. The main energy contributor derives from biogas produced in the anaerobic digester, and heat that is conserved in the wastewater. In certain cases, energy contributions from solar, wind and hydroelectric energy can also be used as follows:

- Biogas - this energy is in the form of a methane-rich biogas that can be extracted and transformed into electrical and thermal energy. If the influent load of organic matter is relatively high, it is easier to extract more energy in comparison with a low loaded plant. The production of biogas occurs where wastewater/sludge is anaerobically treated. Normally, the biogas consists of 60-70% $CH_4$, 30-40% $CO_2$, 4% nitrogen and trace elements. A full scale WWTP in Austria with nutrient removal is energy self-sufficient because the energy production from anaerobic digestion through Combined Heat and Power (CHP) generation is larger than the electrical energy used [82].

- Wastewater heat energy - the stored heat energy in wastewater can be extracted and used for heating WWTPs, as well as distributing to a local district heating network. However, most wastewater plants are located far from urban areas or district-heating networks so the possibility of distributing this to the local district-heating network is limited. Wastewater treatment generally requires the stored heat for enhancing biological activity, so possible heat extraction should occur when the wastewater has already been treated. The wastewater is a suitable heat source because of its generally large volumes and reliable steady flow [66, 83].

- Hydroelectric power - this technology utilizes turbines and/or other devices to generate electricity from effluent water. Such devices may be installed in conduits e.g. pipelines or aqueducts. With the elevation condition, hydroelectric power can be used as an alternative energy source, and commonly a hydroelectric power unit can generate energy with over 70% efficiency. For normal cases, the hydroelectric power can generate a few kW for each metre of height, and the energy generated from this technology is propotional to the flowrate, head, height and generation efficiency. Apart from electricity generation, the effluent hydropower is also able to increase the dissolved oxygen concentration in the treated water. However, the main challenging of this technology is that it requires the effluent to have sufficient kinetic or potential energy to make investment attractive [83].

- Solar and wind energy - solar and wind can be transformed into energy in the form of electricity. A large area of solar panels and wind turbines is necessarily required for extracting energy. Fortunately, most WWTPs cover a large area and the simple shape of the plants makes it easier to install equipment for solar and wind energy generator so these requirements are often satisfied. For the wind energy, most WWTPs are located at a low level and this is a disadvantage when the wind energy aspect is taken into account. In some cases, however, when the plants are placed near the ocean, wind energy can be considered as an interesting alternative. The disadvantage, however, is that solar panels and wind turbines are expensive for investment [84].

### 2.4.2 Resource Recovery

As discussed previously, conventional wastewater treatment facilities are designed to remove organic matter and nutrients from wastewater, rather than resource recovery. Also nutrients, especially nitrogen and phosphorus, are transformed or removed from the wastewater due to their potential to trigger eutrophication or aquatic toxicity. The removal of organic matter and nutrients not only entails energy and/or chemical use, but also often yields byproducts which requires further processing. However, it has been found that wastewater can be a valuable source of resouces rather than a waste. Awareness of this fact has driven the development of resouce recovery technologies, and the following section reviews a number of promising technologies that have been developed for the recovery of energy and materials from wastewater.

#### Energy Recovery

The organic matter in both municipal and industrial wastewater can be transformed into methane-rich biogas through anaerobic digestion. It is estimated that about 30-60 L/d per capita of $CH_4$ could be generated from municipal wastewater if all the biodegradable organic matter was converted into biogas as well as reducing the extra energy cost for aeration used in conventional activated sludge processes [67]. Besides, anaerobic digestion has little effect on nutrient removal, e.g. $NH_4^+$ and $PO_4^{3-}$ so it is a perfect match in terms of resource recovery where nutrients in the effluent can be separated in downstream units.

Biogas generation from wastewater sludge and high-strength wastewater has been commonly used for many years, in contrast to the direct anaerobic treatment of low-strength wastewater, which has not been widely practiced so far, especially in temperature climates where wastewater temperature is in the range of 15 °C. Innovative reactor design has been proposed to maintain elevated biomass inventories, e.g. upflow anaerobic sludge blanket (UASB) and the anaerobic membrane bioreactor (AnMBR), and mitigate some of their limitations, including extending the application range of anaerobic treatment [85, 86]. Promising configurations include the submerged anaerobic membrane bioreactor (SAnMBR; [87, 88]), and the anaerobic fluidized membrane bioreactor (AFMBR; [89]). Research is ongoing to improve membrane and reactor designs that especially reduce membrane fouling and enhance dissolved methane recovery [90, 91] .

In certain water systems where heat accumulates in the wastewater, heat pumps or heat exchangers can be used to recover thermal energy. Although it is low grade energy because of the small temperature differences, this energy only entails low operation and maintenance costs. It is suitable for onsite use, and heating or cooling demands in nearby communities, e.g. for heating buildings. It is estimated that over 500 wastewater heat pumps are in use worldwide, with thermal energies ranging from 10 kW to 20 MW [92].

**Materials Recovery**

Phosphorus is being used in four main applications: agricultural fertilizers (80-85% of all consumption), food or animal feed, detergents and industrial applications. It is a limited resource mainly mined from mineral rock, which has an estimated lifetime of 50-100 years [93, 53]. Consequently, the price of mineral phosphorus has increased, and its recovery from wastewater has now become more economically viable. Phosphorus is generally found in wastewater, especially $PO_4^{3-}$, where in municipal wastewater 50-80% will leave with treated water from where it can be recovered [17]. Nitrogenous compounds, on the other hand, are not a limited resource and can be generated from atmospheric nitrogen, albeit their production is an energy and GHG intensive process. As energy prices increase, nitrogen recovery is becoming a promising alternative, and also its economic viability is increasing. Around 50-80% of the nitrogen in municipal wastewater is present in soluble and inorganic forms [17]. The high content of nitrogen and phosphorus in wastewater can cause eutrophication, reduction of dissolved oxygen levels, and algal blooms which reduce the penetration of solar light. Phosphorus also has a high probability of being precipitated and forming undesired struvites which can block pipes. These blockage can reduce pipe diameter by over 50%, and leads to an increase in energy consumption to pump or drive streams.

Phosphorus and nitrogen ($NH_4^+$, $NO_3^-$ and $PO_4^{3-}$) in wastewater can also be recovered by ion exchange (in contrast to biological methods); the effluent from secondary/tertiary wastewater treatment is passed through ion exchange columns where phosphorus and nitrogen are adsorbed [94, 95]. The columns need to be regenerated cyclically by desorbing both phosphorus and nitrogen with a low volume and concentrated brine solution. The phosphorus and nitrogen enriched solutions can then be processed into a valuable product, e.g. fertilizers. The main advantage of ion exchange over the biological process is that they can be used over a wide range of temperatures. However, challenges with ion exchange are: the potential for fouling with suspended solids, the limited exchange capacity of some adsorbents which require regeneration every few hours, and the limited selectivity due to ion competition for the resin sites and the large capital cost [96]. Natural zeolite, e.g. clinoptilolite to adsorb ammonium ions ($NH_4^+$) has been receiving considerable attention [97, 98], and recently, polymeric resins have been reported as having higher exchange capacities than zeolite [99]. Ongoing research has focused on the development of anion adsorbents with high phosphate selectivity and easy regeneration characteristics, which include polymeric resins with hydrated ferric oxide nanoparticles [100] and hydrotalcite (HTAL) [101].

An interesting alternative for phosphorus recovery is reactive filtration. It combines physical filtration of particulate phosphorus with co-precipitation and adsorption of soluble phosphorus onto coated sand in a moving bed filter. For example, 95% phosphorus removal from secondary municipal effluents could be simply achieved by a continuous backwash filters made of ferric oxide (HFO) coated sand, where continuous regeneneration is applied by adding 5-10 mg/L of ferric chloride ($FeCl_3$) [102]. Then, phosphorus recovery could be achieved with a membrane separator, which receives the backwash from the reactive filter [103] and further processing is needed to convert phosphorus into a saleable form.

Another approach to recovering phosphorus from wastewater is crystallization into reusable and saleable compounds such as struvite ($MgNH_4PO_4{\cdot}6H_2O$) and calcium phosphote $Ca_3(PO_4)_2$ [55]. Struvite is, however, in the preferable form for fertilizers because Mg, N, P can be simultaneously released with 1:1:1 molar ratio, and the rate of nutrient release is slower in comparison with other fertilizers; this technology involves precipitation in either fluidized bed reactors or stirred tanks [104]. The former is commonly used to crystallize struvite from wastewater, and the applications to date have been used to extract struvite from sludge digester liquor produced from anaerobic digesters due to high concentration of phosphorus (50-100 mg/L of phosphate), $NH_4^+$ and Mg in them. Under well-controlled conditions, removal efficiencies of 80% or higher have been reported [105]. When dilute streams, such as secondary effluents with phosphate concentrations of 4-12 mg/L are considered, struvite crystallization can be combined with adsorbent columns and fed with enriched solutions from the adsorbent regeneration; such as in the RIM-NUT® process by Liberti et al. [95]. A struvite crystallization plant has been operated at several locations in Japan since 1987, with capacities of 100-500 kL/d, and produce from 100-500 kg/d of struvite. There are also three full scale plants which are currently operated in the US. However, most of current studies are on pilot scale in Australia, Canada and Spain.

In addition to nutrients, organic carbon recovery can be achieved through the production of polyhydroalkanoates (PHAs), a precursor of bioplastics [106]. PHAs are linear polyesters produced from the fermentation of sugars or lipids by bacteria as energy storage (up to 50% weight). Their production is technologically proven from synthetic wastewater under well-controlled conditions. However, full-scale applications are still at the embryonic stage, in part due to the challenge associated with the separation of PHAs from the bacterial biomass. It should also be clear that PHA production, when used in combination with anaerobic digestion, will result in a net reduction of biogas production by the digester since it diverts part of the available organic carbon.

## 2.5 Review of WWTP Modeling

The concern about sustainability issues has encouraged researchers in the wastewater community to focus on the proper design, operation and control of WWTPs. The performance of WWTPs varies from one plant to another, and this gives rise to adverse environmental, cost and public health risks due to improper operation of WWTPs. However, optimal design, operation and control of WWTPs can be achieved though using modeling tools which represent the real system, and can be used as a decision-making tool [107]. The usefulness of the model is independent of its completeness, but it is more important to select the model based on its intended use [108]. Mathematical modeling of wastewater treatment processes is becoming a widely accepted tool, and used for several purposes in the wastewater treatment process, especially for process design [109], control and operation [108]. There are a number of models describing the processes in WWTPs, starting from activated sludge through to whole plant models. Most of the models of wastewater treatment processes are incorporated into commercial simulation packages e.g. BioWin®, GPS-X®, WEST® and STOWA. Currently, the design, upgrading/retrofiting of WWTPs and improvement of process operation are based on simulation results. More plant engineers and operators are now being trained to use the mathematical models as decision-making tools because it is easier for them to assess the outcomes of the process modification on WWTP performance and/or effluent quality.

### 2.5.1 Modeling in WWTPs

Over the last two decades, mathematical modeling of WWTPs has been divided into three main areas. Firstly, the wastewater stream including nutrient removal has been investigated; this group is dominated by Activated Sludge Models (ASM) models developed by the International Water Association (IWA) [110] to predict the organic matter and nutrient removal from the wastewater stream. The second group involves modeling of sludge stabilization, which is dominated by anaerobic digestion processes, and the IWA ADM1 model. The final group is modeling of the whole WWTP which considers all wastewater streams, sludge streams and the recycle stream which results in significant nutrient loads on the overall WWTP from sidestreams.

#### 2.5.1.1 Activated Sludge Model

The biological phenomena involved in aerated bioreactors are modelled by the activated sludge model. Over the last thirty years, four activated sludge models known as the ASM models (i.e. ASM1, ASM2, ASM2d and ASM3) have been published by the IWA (International Water Association) [110]. These models are widely used to describe the behaviour of activated sludge processes, and all of these models are based on the same principles; the biological activities in the activated sludge process are described through different compounds (substrates, particulates and biomass), and a number of processes based on mass conservation equations. The reactions of different processes rely on the concentration of compounds/biomass by using Monod equations. The models are typically summarised in a matrix format (Petersen Matrix) where the processes are represented in rows, and the components in columns and the stoichiometry in the table. An example of ASM1, which is represented in the Petersen Matrix format, is shown in Table 2.2. See the IAWQ Task group reports [110] for further detail.

Table 2.2: Example of ASM1 in the Petersen matrix format [111].

| Component, i → | 1 | 2 | 3 | 4 | 5 | Reaction rate |
|---|---|---|---|---|---|---|
| Process, j ↓ | $S_I$ | $S_S$ | $X_I$ | $X_S$ | $X_{BH}$ | |
| 1. Aerobic growth of heterotrophic bacteria | | $-\frac{1}{Y_H}$ | | | 1 | $\mu_{mH}(\frac{S_S}{K_S+S_S} \cdot \frac{S_O}{K_{OH}+S_O})X_{BH}$ |
| 2. Anoxic growth of heterotrophic bacteria | | $-\frac{1}{Y_H}$ | | | | $\mu_{mH}(\frac{S_S}{K_S+S_S} \cdot \frac{K_{OH}}{K_{OH}+S_O} \cdot \frac{S_{NO}}{K_{NO}+S_{NO}})\eta_g X_{BH}$ |

ASM1 was first developed by Henze and co-workers [111], and the main activities occurring in the bioreactor include oxidation of organic compounds, nitrification/denitrification, decay of the biomass, the ammonification of soluble organic nitrogen and hydrolysis of particulates. It is based on 13 components: particulate-soluble inert compounds ($X_I$ and $S_I$), particulate-soluble substrate ($X_S$ and $S_S$), autotrophic/heterotrophic biomass ($X_A$ and $X_H$), particulate inert compounds from biomass decay ($X_P$), oxygen ($S_O$), ammonium/ammonia ($S_{NH}$), nitrate/nitrite ($S_{NO}$), particulate-soluble organic nitrogen ($X_{ND}$ and $S_{ND}$) and alkalinity ($S_{alk}$).

Several extensions of the ASM1 model have been developed later on, which add a number of processes or fix certain limitations. The ASM2d model encompasses biological and chemical phosphorus removal, based on the following fractionation (Note that fractionation is refered to concentration of the wastewater characterisation components used to describe wastewater characteristics. For example, ASM1 consists of 13 wastewater characterisation components used to describe composite components, e.g. COD, TSS and TN.); phosphate ($S_{PO_4}$), phosphorus accumulating biomass ($X_{PAO}$), internal cell storage ($X_{PHA}$), poly-phosphate ($X_{PP}$), metal-hydroxides ($X_{MeP_4}$) and metal-phosphate ($X_{MeP}$). Moreover, soluble organic substrates are further divided into fermentable substate ($S_F$) and fermentation products ($S_A$) with a fermentation process describing the transition between two substrates. However, ASM1 remains the most commonly used activated sludge model in the literature due to its rather low complexity, extensive calibration, and the lack of trust in other models. More recently, several studies have focused on the mechanisms and conditions that trigger $N_2O$ emissions. The activated sludge model-nitrogen (ASMN) model developed by Hiatt and Grady [112] is an extension of ASM1 with two-step nitrification and four-step denitrification, capable of quantitative prediction of $N_2O$ emissions from these intermediate processes.

#### 2.5.1.2 Anaerobic Digestion Model

In the early 70s, modeling of the anaerobic digestion process started in order to improve the efficient operation of anaerobic digesters. Due to a limited knowledge of the process, the models in that period were relatively simple [113]. With the development of system analysis and computing capabilities, more detailed models have been developed in recent years. The generic model, Anaerobic Digestion Model No.1 (ADM1), developed by the IWA Task Group for Mathematical Modeling of Anaerobic Digestion Process [114] is one of most widely used for describing anaerobic digestion among alternatives. The ADM1 includes 24 components and 19 bioconversion processes to describe the dynamic anaerobic digestion, as illustrated in Figure 2.10. The model involves biochemical processes (hydrolysed by intra-extra cellular enzymes) and physico-chemical processes (gas-liquid transfer and ion association/dissociation); however, precipitation is not included in the model. The degradation sequence of organic matter for anaerobic digestion is shown in Figure 2.10. The complex compounds are firstly hydrolysed into carbohydrates, proteins, lipids and inerts (i.e. not degraded further during anaerobic digestion). Then, carbohydrates, proteins and lipids are hydrolysed by enzymes into monosaccharides, amino acids and long chain fatty acids (LCFA), respectively. The next step is known as acidogenesis in which monosaccharides and amino acids are degraded into acetic, propionic, butyric, valeric acids and hydrogen. After that, it is the action of acetogenesis where propionic, butyric, valeric acids and long chain faty acids (LCFA) are degraded into acetic acid and hydrogen. Finally, two groups of methanogenic bacteria degrade acetic acid and hydrogen to $CH_4$. All of these reactions are first order kinetics, which are regulated by the Monod equation relevant to the substrate, inihition, hydrogen and free ammonia. The large number of parameters, difficult identifiability, and structural weaknesses are the major drawbacks of ADM1, although it has been used in many applications in recent years

[115, 116].

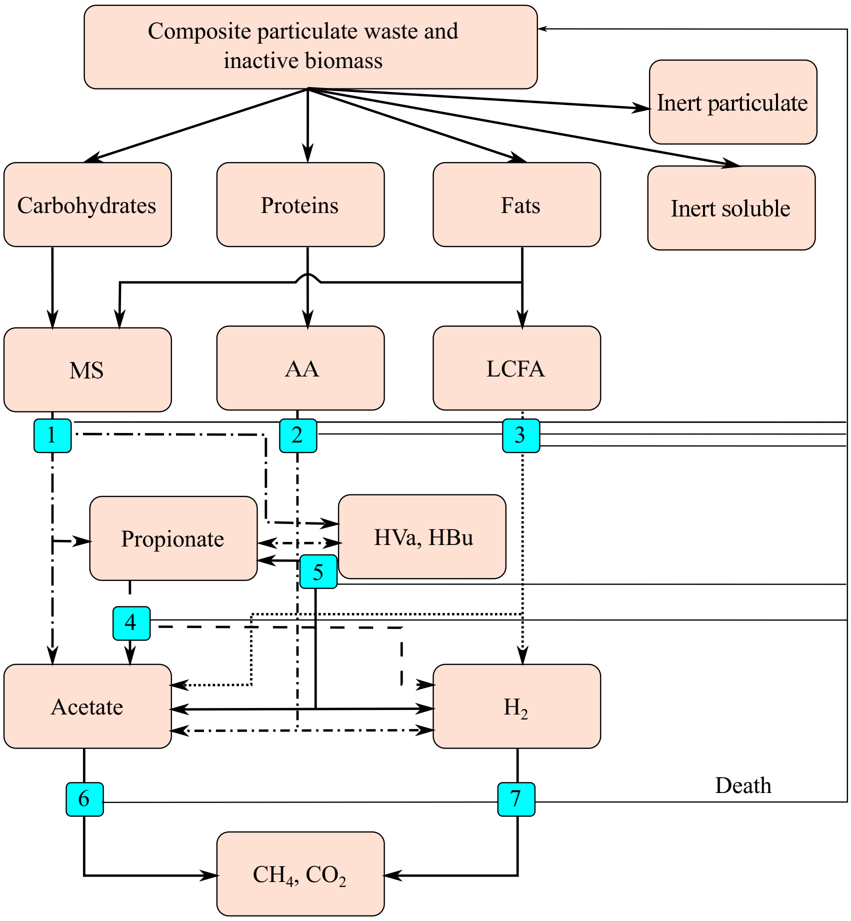



Figure 2.10: Schematic representation of processes in the ADM1: (1) acidogenesis from sugars, (2) acidogenesis from amino acids, (3) acetogenesis from LCFA, (4) acetogenesis from propionate, (5) acetogenesis from butyrate and valerate, (6) aceticlastic methanogenesis, and (7) hydrogenotrophic methanogenesis modified from Batstone et al. [114].

#### 2.5.1.3 Plant-wide Model

Recently, more attention in the wastewater treatment community has focused on the modeling of the whole WWTP, which considers both wastewater and sludge streams. WWTPs involve a great variety of processes acting on different time scales, and interacting with each other through recycling loops. Although it is more convenient to study an individual process, a whole plant should eventually be considered for a number of reasons: i) even processes in a simple sequence are often affected by the previous process, e.g. utilization of COD and biomass, and; ii) interactions between the processes can propagate the effect from one process to the next through recycle streams [108]. As a result, the design and operational policy of an entire WWTP may differ from the compilation from a unit-process. Modeling of plant-wide WWTPs is not a straightforward task [117] because the existing standard models have been focused mostly on development of the individual unit process. This gives rise to considerable inconsistencies and differences in model components and transformations among the standard process models in terms of descriptions of carbonaceous substrates, nitrogen, pH and buffer capacity [118].

Up until now, two main approaches have been proposed to handle modeling of the whole WWTP: the supermodel and interface approaches. For the supermodel, a common fractionation to reproduce every process within the WWTP is developed to describe the biochemical, chemical, physico-chemical or relevant processes of the whole plant [119]. It is convenient to use this approach because no transformation is required between unit process models, and the transformations can be simply turned on/off depending on the environmental conditions. However, the main drawback of this approach is that the supermodel lacks flexibility to add or remove components, and may need to develop a new model when a new process is added. Additionally, supermodels are not fully documented in the literature and are restricted to specific simulation platforms, e.g. the Activated Sludge Digestion Model (ASDM) in BioWin® [120, 121].

An extensive supermodel was proposed by Grau et al. [118]; this approach includes only the most relevant transformations and components, instead of listing a priori the required fractionations. The descriptive capacity of the models, the complexity of mathematical formulation, and the number of components are adapted to the specific objectives and requirements of the plant. Even though some of the models can turn on/off blocks of transformations, this approach is based on user selection from a set of transformations which is strictly required to reproduce the activity of the related bacterial populations in the WWTP. Therefore, the availability of a consensus and common transformations which includes all relevant process transformations is an important aspect of modelling.

This approach is more flexible in constructing the supermodel than the previous approach, which are specificially modified/adapted to the plant requirements. However, a rigorous and systematic way to select transformations to create the appropriate model for a specific case is needed.

The second method is known as the interface approach, and is based on the construction of specific interfaces to connect the existing standard unit process models; the interface transformation converts one set of fractionation to another. The equation of continuity of the mass and charge balances are included in the tranformations to make sure that it is consistent from unit to unit. For instance, the ASM1-ADM1 interfaces were proposed to link the activated sludge model no.1 (ASM1) and anaerobic digestion model no.1 (ADM1), and Nopens et al. [122] developed an interface and characterisation model. Degradable components from ASM1 are mapped directly to carbohydrates, proteins and lipids, as well as organic acids instead of using pooling techniques in terms of $X_C$ proposed by Copp et al. [123]. The main advantage of this approach is that each unit-process model is quite standard and has been successfully applied to many practical case studies. However, model components, e.g. COD fractions, description of organic nitrogen, pH and alkalinity are different from process to process. Up until now, plant-wide modeling is still discussed in the scientific community because there is no general consensus on the simplest modeling approach. The current approach used by most researchers is still based on personal preferences and modelling software capabilities.

### 2.5.2 Model Applications in WWTPs

Modeling of WWTPs is practically used in two main applications: i) process control and optimisation where several scenarios are evaluated to improve operation of existing WWTPs and ii) process synthesis and design where several WWTP configurations are screened and assessed.

#### 2.5.2.1 Process Control and Optimisation

Over the past few decades, tighter effluent limits imposed on WWTPs, and enhancing sustainability have been the driving forces to improve treatment technologies, and these need both process control and optimisation. Modeling is a valuable tool in terms of time and effort required to predict different what-if scenarios to push WWTPs toward sustainability. The benefits of process control and optimisation in WWTPs range from improving WWTP performance and energy saving, while effluent quality is satisfied. Proper control and operation of WWTPs have been receiving more attention recently because of the rise in energy prices, and environmental concerns. Inadequate strategies for process operation of WWTPs may lead to an increase in energy use, and serious environmental/public health problems [124]. The use of modeling for process control and optimisation can be applied both online and offline; the former refers to the use of calibrated models for on-line schemes such as model predictive control [125], and a plant-wide control system [80, 126]. The latter is used in applications where the calibrated model is used to determine optimal conditions, and the results are later applied and tested on real plants. Process control and optimisation have been used for several purposes, and most studies have evaluated different scenarios through simulation. For instance, new stricter regulations are applied to the existing WWTP, or significant changes in the plant loads. Based on the current operational or control strategies, the effluent quality may not satisfy the new regulations, or it requires more energy expenditure. The model can be used to evaluate new operational and control strategies to improve the existing plant, which is typically carried out through process simulation [127, 128, 129, 130, 131, 132, 133, 134, 135].

Some studies have focused on the evaluation and comparison of plant-wide WWTP control strategies to improve process performance in terms of economic and environmental objectives. In the wastewater treatment community, improvement of control and operational strategies through the DO setpoint in activated sludge has received considerable attention. This is because aeration and pumping have the largest impact on the energy cost in WWTPs, and reliable effluent quality is expected to be maintained at reasonable cost despite disturbances [136]. Pittoors et al. [136] found that model-based aeration optimisation can lead to alarge cost reduction of up to 66%. In addition, some attention have been paid to sustainability issues in WWTPs, including the use of models to evaluate energy consumption, chemical use, and GHG emissions. Few attempts have also been made to combine GHG emissions with the plant performance; Guo et al. [137] proposed a benchmarking tool to evaluate mitigation strategies to reduce fugitive emissions by means of a generic sewer model, including a WWTP plant-wide model. The new activated sludge model for GHGs (ASMG) was implemented and used to predict direct nitrous oxide ($N_2O$) emissions from biological treatment, while other GHG emissions were obtained through empirical relationships. Different scenarios were then tested to compare performance in terms of GHG emissions, effluent quality and energy consumption. Flores-Alsina et al. [138] investigated the effect of changing control/operational strategies in WWTPs on the plant performance, which included GHG emissions, effluent quality (EQI) and operational cost (OCI). The GHG evaluation was based on dynamic models that included both on-site and off-site sources of $CO_2$, $CH_4$ and $N_2O$. The process variables under study consisted of the set point for aeration control in the activated sludge, the removal efficiency of TSS in the primary settler, the anaerobic digestion temperature, and the control of the supernatant flow from sludge treatment. Their results showed the potential impact of energy efficiency, particularly in the importance of plant-wide evaluation, energy reduction in the aeration system, and energy recovery in anerobic digestion. However, the beneficial impacts were counterbalanced by an increase in $N_2O$ emissions. For instance, decreasing the DO setpoint may reduce the offsite $CO_2$ emissions due to a decrease in electricity use, but the $N_2O$ emissions also increase significantly. The authors also emphasized the advantages of using multiple criteria as a decision-making tool to evaluate the control/-operational strategies.

Recently, many optimisation approaches for process design and operation have been improved and are available in the scientific literature. Each method has several advantages, but also drawbacks which can limit their potential; gradient-based methods offer a promising approach among alternatives. It can provide a high level of precision and rapid convergence to the optimum, and this approach has been applied to a WWTP under steady state and dynamic conditions. The reactions in the wastewater treatment process involve a wide range of time scales from less than a minute, e.g. the dissolved oxygen concentration to several days, e.g. the growth of biomass. Thus, the dynamic model accounting for the time-varying responses of the system can be defined differently based on the objectives. Gradient-based optimisation has mostly been applied to small-scale WWTPs [139, 140, 141, 142], while Rivas et al. [109] presented a model-based decision making tool for predicting optimum design parameters in a WWTP. The proposed mathematical model can be solved using a non-linear optimisation algorithm (GRG2), which can be applied to either a steady state or dynamic model under a set of constraints associated with operation and effluent quality. The proposed methodology was applied to simple case studies to evaluate the optimum design parameters, e.g. HRT, SRT, and volumes for the activated sludge Step-Feed process to enhance nitrogen removal. The Step-Feed process is an approach to remove nitrogen by using a couple of stages of denitrification-nitrification in series. The influent flow is distributed to the anoxic tanks which can increase the suspended solids gradient through the reactors; the main advantage of this approach is that internal recycle of the mixed liquor is not required.

However, only a few articles have applied the plant-wide model-based methodology for process optimisation. Descoins and coworkers [143] optimised a whole wastewater treatment process by evaluating the electrical efficiency. In this work, the WWTP configuration is based on the plant-wide BSM2 model, including activated sludge and anaerobic digestion, to identify the optimal operating conditions. In order to satisfy the standard regulations, wastewater with a high content of nitrogen needs to be treated through nitrification/ denitrification which consume large amounts of energy. Sludge from primary and secondary treatment is sent to the anaerobic digester to produce a methane-rich biogas. Although anaerobic digestion can produce a methane-rich biogas, it also produces more $NH_4^+$ from the degradation of organic matter which is then sent back to the activated sludge process. Thus, trade-offs between energy consumption for nutrient removal and electricity produced from biogas were performed through plant-wide optimisation. The methodology of plant-wide modeling was based on a new plant-wide modeling as proposed by Grau et al. [118], and the model was simulated/optimised on the gPROMS platform under steady state conditions. Their results showed that there are strong links between nitrogen removal, availability of carbon substrate for denitrification, and overall electrical efficiency. It is also possible to select the optimum point of primary settling efficiency and the amount of carbon needed for denitrification.

#### 2.5.2.2 Decision-making Tool for Process Design

Similarly, upgrading existing WWTPs and/or the design of new wastewater treatment facilities can be carried out by means of modeling. The modeling approach offers a substantial reduction in time and cost during scaling-up the processes; for instance, different wastewater treatment processes can be evaluated in terms of cost analysis and/or environmental impacts before building a pilot plant. Typically, it can transform useful data obtained from measurements into quantitative knowledge which can be further used in the decision-making processes. As a result, it is used to close the discrepancies between lab-scale experiments and full-scale implementations to select the desirable wastewater treatment systems [144]. In recent years, a number of wastewater treatment technologies have been developed to address current and future conditions, i.e. the effluent from WWTPs needs to satisfy the Urban Wastewater Treatment Directives (91/271/EEC). No single or group of technologies, however, have been developed to satisfy all conditions that may occur within these systems. As a result, different technologies or treatment units are combined and modified to satisfy the specific requirements [145]. The number of technologies developed has steadily increased the number of possible process configurations, which makes it more and more difficult to select the optimal wastewater treatment process flowsheet. The traditional approach to process design of WWTPs is based on engineering calculations and empirical knowledge, e.g. Metcalf & Eddy [17], which may not be adequate for these emerging new technologies such as SanMBR, and the targets they have to achieve.

Hamouda et al. [18] reviewed and summarized approaches to developing decision-making tools in the process design of WWTPs. Typically, there were four stages to developing decision-making tools for the WWTPs. Firstly, it involves the problems analysis, which may be concerned with specific contaminants or treatment processes; there are generally several factors which need to be considered when selecting the wastewater treatment processes. Technical and economic aspects such as removal efficiency, and capital cost are commonly used because they are easier to quantify and compare among various alternatives, while different factors can provide different insights about the characteristics of the wastewater system. However, the integrated system including economical, technical, social aspects is more reliable and sustainable as it can account for interactions among the various system components. The second stage includes development of reasoning models where knowledge can be collected from the previous stage, and relavant data can be extracted from different sources, such as the literature and case studies. Several approaches can be used to acquire knowledge, e.g. mathematical programming, simulation and artificial intelligence; selecting the best approach is based on type, available knowledge and a set of objectives. Later, the actual decision-making process is used to evaluate different alternatives for process selection in the third stage. The optimisation approach is an important aspect at this stage, and needs to incorporate all the criteria to select the best possible option. In the final stage (fourth stage), usability is required through validation and verification to make sure that the results obtained are meaningful, correct and consistent.

Mathematical modeling has been a powerful tool to assisting decision making in WWTP design since the 1990s. Not only have the computational capabilities and numerical solution technology improved drastically, but the mathematical models too have become more predictive, now enabling plant-wide simulation routinely using a range of commercial simulators (GPS-X®, BioWin®, WEST®, etc). Conventional model-based WWTP design starts with the selection of a plant layout, and then focuses on the detailed design and analysis of this particular layout. The selection of an appropriate design that meets the specified objectives and constraints involves comparing the capital and operating costs of multiple plant configurations, thus requiring repetitive model simulations alongside comprehensive process knowledge. As the number of processes and configurations increases, this design approach becomes more tedious, and ultimately unmanageable.

In order to deal with large numbers of treatment or separation units and possible interconnections, a system engineering approach defined as the interdisciplinary approach or development of systematic methods for design and operation of the complex process systems is most useful. Systematic methods for the synthesis of complex chemical plants and biorefineries based on superstructure modeling and optimisation are well developed [19, 146, 147]. These approaches are also increasingly applied to water network synthesis in process plants in order to minimize fresh water consumption and wastewater generation through regeneration, recycle and reuse [20, 23]. Regarding municipal wastewater facilities, the need for systematic approaches has been emphasized [10, 18], but relatively few studies have been published to date [26, 25, 148, 28]. These studies provide insight into the potential of the systematic optimisation-based approaches for wastewater treatment design, but they are nonetheless limited to optimising a given process or selecting the most appropriate process among a small number of alternatives mainly based on economical considerations.

### 2.5.3 Model Calibration

Modeling in WWTPs is useful for process design and operation, however, it is important for models to be calibrated for reliable and correct representation of the real system. Model calibration is defined as the adjustment of the model parameters, e.g. influent fractionation, stoichiometric and kinetic parameters, to fit a certain set of data obtained from experiments and/or measurements of full-scale applications. Several protocols for model calibration have been developed by different research groups over the last few decades, however, it is still the main bottleneck in wastewater modeling. Model calibration is a challenging task as models, especially biological processes, are complex and typically characterized by a large number of variables and parameters [149]. Also, there are a number of model outputs that need to be fitted with the limited measured data in terms of effluent quality. As a result, wastewater models are over-parameterized and there are generally problems with identifiability; hence, unique estimation of all parameters is not possible, although selected parameters can be used for fine-tuning the model calibration. Note that input data including influent wastewater and operational data are expected to be checked and elaborated carefully before introducing them into the model. Reliable measurement is required over a period of time from a few days to years to capture steady state and dynamic behaviour in the WWTPs. Up to now, parameter selection has been carried out through: i) an experience-based approach, which use process knowledge and experience, and, ii) a systems analysis approach where the identifiability of the model is based on the sensitivity analysis of model parameters [150]- both approaches have different advantages and disadvantages. It is worth pointing that the experience-based approaches based on engineering knowledge and cumulative experience has been most commonly used in the wastewater treatment field. In contrast, applications have been limited for the system analysis approach in this field [150].

With respect to the experience-based approach, expert knowledge and experience are important. Calibration protocols require some experimental designs, as well as data analysis to reduce the number of calibrated parameters, and certain parameters, e.g. batch tests are fixed to obtain accurate or reasonable predictions. Sin et al. [151] reviewed four different calibration methodologies: Biomath [152], STOWA [153], HSG [154] and WERF protocols [155]. These calibration protocols have common points in terms of: i) influence of goals in the calibration, ii) the importance of data collection, verification and reconciliation, and iii) the suggestion of validating the model with a different data set. However, these approaches are different based on three main points: i) the planning of the measurement campaign; ii) the measurement approach to characterizing wastewater influent, and; iii) the calibration approach including the selection of parameter subsets. The system analysis approach has attracted more attention, and includes a sensitivity analysis, parameter identification and error propogation. The parameter subset for model calibration is selected based on a sensitivity analysis which can be performed through either local or global techniques. Identifiability measures are then evaluated from a subset of parameters ranked in the previous step. Although several models and calibration protocols have been developed extensively, only a few studies have applied such concepts to full-scale WWTPs.

Liwarska-Bizukojc et al. [156] presented the calibration results for a full scale WWTP in Poland serving a community of 94,000 population-equivalents. It consists of three zones of biological treatment and clarifiers in the Phoredox process configuration, which is a sequence of anaerobic, anoxic and aerobic zones. The data were collected to perform steady state (1 month) and dynamic calibrations (48 hr) and analysed through a statistical analysis. The model was implemented in the commercial wastewater treatment process simulation, BioWin®. Prior calibration, and a sensitivity analysis, including the calculation of a normalized sensitivity coefficient, was investigated to rank the sensitive parameters to use for calibration purposes. Most of the highly sensitive parameters were associated with the growth and decay of ordinary heterotrophic bacteria and phosphorus accumulating bacteria. The results from the model calibration revealed that there were no statistical differences between the simulated results and the measured data for steady state; however, discrepancies of up to 20% could be observed from the dynamic calibration.

However, traditional plant operation provides only routinely measured data such as BOD, COD and TSS, which may not be directly applicable for modeling purposes. There are only a few examples in the literature where only plant operating data was used [157], and Sochacki et al. [158] used the plant-wide modeling approach in a full-scale WWTP in Poland. Model development and calibration were based on only routinely obtained operational data from the WWTP, without additional measurements. The WWTP consisted of primary settling, four activated sludge bioreactors, a secondary clarifier, thickener and anaerobic digester. In this study, the plant-wide model was implemented in the commercial wastewater treatment process simulator, WEST® and model predictions use effluent quality, biogas production and input sludge concentration in the anaerobic digestion as the indicator of model accuracy. The results show that the calibrated model can provide acceptable accuracy with limited data, however, there was still limited predictive ability, and the model represents only specific variables.

## 2.6 Summary of Current Studies and Research Objectives

Conventional WWTPs have been used for many years to treat wastewater before discharge into receiving water bodies to protect both the environment and public health. However, they are energy-intensive and it is likely that energy use will increase significantly in the future due to increasing population and stricter discharge regulations. In addition, GHG emissions and sludge disposal are critical issues that can exacerbate these problems in the future. These are the main driving force for the improvement of existing WWTPs and development of new wastewater treatment facilities to achieve sustainability. Based on the foregoing review which presents a general background and current studies in the wastewater treatment field, this section outlines the gaps in the literature summarised as follows:

**Improvement of Existing WWTPs**

Plant-wide model-based methodology has been used as a tool in several applications, e.g. evaluating control and operational strategies when stricter regulations are applied or investigating effects of changes in the plant loads. However, few studies have applied the plant-wide approach to full-scale WWTPs. Mannina et al. [149] pointed out that model applications to a full-scale WWTP is a challenging task due to the fact that there are a number of model parameters that need to be estimated compared to the limited data. A major challenge here is to develop a reliable plant-wide model with the limited amount of plant data that is typically available. In addition, incorporation of GHG emissions with effluent quality and operational cost as performance indicator is another challenging task. It is important to point out that there is a trade-off between energy consumption, effluent quality and GHG emissions. Thus, a decision support tool is needed to identify or balance trade-offs between effluent quality, operational performance and GHG emissions.

**Development of New Wastewater Treatment Facilities**

To date, decision-making tools for design of wastewater treatment facilities is not fully developed. Conventional WWTP design is based on experience and engineering guidelines [17]. It is interesting to point out that model-based WWTP design is mostly based on the pre-selection of plant-layouts and simulation of the selected plant configurations. Then, each WWTP configuration is compared in terms of the capital and operating costs to choose the most appropriate design [109]. As the number of process and configurations increases, this approach is becoming more difficult and unmanagable. Some studies have investigated using the optimisation-based approach [26, 25]. These studies can provide insights to select the promising WWTP but the concept is limited to either optimising the best process configuration from a small number of alternatives or given treatment process. A major challenge here is to use a systematic approach to select the most promising and optimal wastewater treatment facilities among process alternatives. Additionally, most WWTP design studies aim to minimise the contaminants in wastewater but do not consider the overall environmental impacts. As a result, it has negative impacts on the overall environment. LCA methodology should be incorporated with economic and social evaluations to provide a more complete picture of sustainability [159]. Therefore, it is important to link the economic and environmental criteria to address problems regarding sustainability and to achieve wider acceptance amongst decision-makers.

**Research Objectives**

Based on the research gaps summarized previously, the specific research objectives addressed in this thesis are the following:

- To develop a better understanding of what level of nutrient discharges, energy consumption and GHG emissions can be reduced and what impact further reduction in nutrient discharges has on the overall plant's performance. This information can be used to identify the main trade-offs between effluent quality, energy consumption and fugitive emissions.
- To investigate the feasibility and assess the potential of systematic (model-based) optimisation methods for enhancing the removal of nutrients and reducing the energy consumption in existing wastewater treatment facilities.
- To develop a superstructure optimisation methodology for synthesis of sustainable wastewater treatment/recovery plants using plant-wide surrogate models, and to demonstrate computational tractability using state-of-the-art optimisation technology that can provide a certificate of global optimality.
- To develop a decision-making tool for the synthesis of sustainable wastewater treatment/recovery facilities with biosolid management that incorporates Life Cycle Assessment (LCA) alongside economic criteria.

# Chapter 3

# Plant-wide Model-based Assessment of WWTP Operation

## 3.1 Introduction

WWTPs have conventionally been assessed through effluent quality, subject to technical feasibility and cost, but the issue of sustainability as defined in Chapter 1, especially GHG emissions, is becoming increasingly important. This is because significant amounts of GHGs are emitted from full-scale WWTPs [160]. In addition, control and operational strategies of WWTPs are traditionally set to maintain suitable effluent quality even with unpredictable events, such as heavy rainfall and/or high loading contaminants. One drawback of such operational strategies, however, is that it not only entails high operational costs, but it can also have large environmental impacts due to $CO_2$ and other fugitive emissions, mostly from electrical power consumption. Analysis of overall impacts on the environment is rarely available because WWTP performance is generally assessed based only on its point-source discharge to a water receiving body. However, increasing demand for environmental protection at a lower cost, together with concerns about GHG emissions, are important driving forces to enhance the sustainability of existing WWTPs.

Among the various alternatives for the sewage industry to reduce their energy consumption, and other environmental impacts, without compromising on effluent quality is improving the control and operational strategies of the WWTP. These strategies may be particularly useful for energy intensive processes such as activated sludge aeration, which can account for 45-75% of a plant's energy expenditure [67]; overall, it is estimated that energy consumption of most WWTPs could be reduced by 10-40% [161]. Nonetheless, WWTPs are comprised of a large number of treatment and separation units, which involve a great variety of processes acting on different time scales and interacting with each other via recycling loops. Failure to account for these interactions, for instance, by considering optimisation in a unit-wise manner, may not lead to the largest possible improvements, and could even be detrimental to the overall efficiency [143]. In this context, developing effective operational strategies can defy engineering intuition, and plant-wide simulation models, such as BSM2 [116], have started playing an increasingly important role [138, 143] in investigating optimal operating strategies.

Plant-wide mathematical models have been used to consider interactions between processes, and to investigate and compare the performance of different operational strategies. Thanks to a better understanding of the chemical and biochemical mechanisms of GHG emissions, several research groups in the wastewater community have developed the mathematical models to predict GHG emissions from WWTPs, and/or incorporate the capability of GHGs e.g. $CH_4$, $N_2O$ and $CO_2$ predictions into the existing standard models [112, 162]. However, only a few studies have discussed the practical benefits of adding GHG emissions as a criterion together with effluent quality and operational costs for performance evaluation [138]. The study of Flores-Alsina et al. [138] presented the considerable advantages of including GHG emissions as the additional criterion to evaluate different control strategies through four key operating variables: the DO set-point, removal efficiency of TSS in the primary sedimentation, the temperature in the anaerobic digester and the flowrate of supernatants from anaerobic digesters. A shortcoming is that they did not quantify what level of nutrient discharges, energy consumption and

GHG emissions can be reduced due to the limited number of scenarios. Also, one of the $N_2O$ emission pathways through incomplete oxidation of hydroxylamine to $NO_2^-$ was not taken into account and did not deal with model calibration to the WWTPs which is a challenging task as pointed out by Mannina et al. [149].

The main contribution and novelty of this chapter is to apply a model-based methodology to provide a better understanding of how changing the effluent quality targets impacts on plant-wide energy use and fugitive emissions. More specifically, the developed model can used to identify what level of nutrient discharges, energy use as well as GHG emissions can be reduced and what impact further reduction in nutrient discharges has on energy use and GHG emissions, e.g. a significant increase of energy use and GHG emissions. With the application of the scenario-based simulation, it will help assess more precisely the potential of operational strategies upon relaxing certain discharge limits. This chapter is related to developing a reliable plant-wide model based on the commercial simulator BioWin® and gPROMS, and calibrating the plant-wide model to predict the performance of an activated sludge plant with sludge treatment owned and operated by Sydney Water. A scenario-based approach is then applied to quantify the effect of key process variables, and to identify operational strategies that reduce energy consumption and fugitive emissions at different nutrient discharge levels. These operational improvements are also compared to an alternative plant upgrade scenario based on reverse osmosis to achieve a better effluent quality. This improved understanding of the relationship between energy use and nutrient removal will feed into discussions with environmental regulators regarding nutrient discharge licensing. The remainder of this chapter is organised as follows: Section 3.2 focuses on the methodology to set up a reliable plant-wide model to predict performance, energy consumption and GHG emissions. Section 3.3 presents results of the model calibration and validation, based on data derived from routine and non-routine measurements, to ensure that the plant-wide model can represent the actual system. This also includes results of a plant-wide analysis through model predictions with different operational strategies.

## 3.2 Methodology

### 3.2.1 Plant Description

The WWTP under investigation is a tertiary plant owned and operated by Sydney Water. Over the years, the pollution load on this WWTP has increased significantly, and its effluent discharge constitutes a main point source of pollution for the receiving surface water. The general layout is shown in Figure 3.1; it operates two parallel primary/secondary treatment lines, called Stage 1/2 and Stage 3 hereafter: Stage 1/2 operates a primary clarifier followed by a Bardenpho process (a Modified Ludzack-Ettinger (MLE) process followed by a sequence of anoxic and aerobic zones) to remove total nitrogen (TN); Stage 3 operates an A2O process to remove both TN and total phosphorus (TP) using primary sludge from Stage 1/2 in the initial anaerobic zone. These parallel stages are followed by a common tertiary treatment for effluent polishing, while the secondary sludge is digested aerobically before disposal. The nutrient discharge limits currently in application are 5 mg/L, 45 mg/L and 5 mg/L for $NH_4^+$, TN and TP, respectively, although a much higher effluent quality is produced. This WWTP is flexible enough to explore a wide range of scenarios and presents excellent potential for optimisation due to substantial interactions between its two treatment lines.

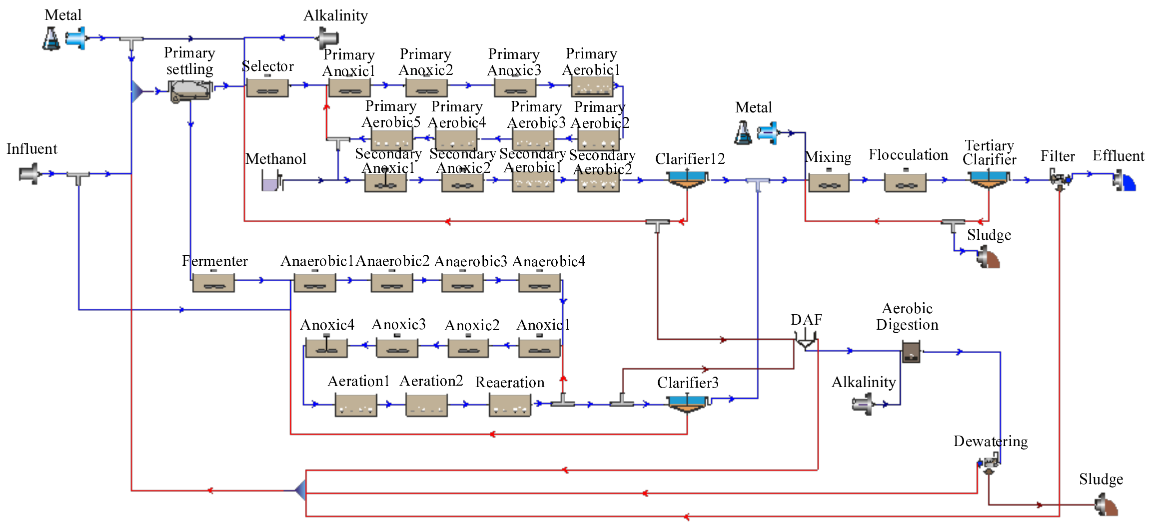



Figure 3.1: Activated sludge plant layout.

### 3.2.2 Data Acquisition

Historical data is routinely collected from both online measurements such as daily flow, pH and dissolved oxygen, and from laboratory analysis of an extensive range of biological and chemical parameters. The laboratory analysis is carried out onsite at the WWTP, and at a laboratory accredited by the Australian National Association of Testing Authoritis carrying out analyses such as COD, $BOD_5$, TSS, N-$NH_4^+$, N-$NO_3^-$ and TN. Moreover, additional data collected from a two-week non-routine monitoring campaign (conducted in June and July in 2013) were used for model calibration, and 12 months of data (from April 2012 to April 2013) from Sydney Water's data management system for the model validation.

The collected data for model calibration and validation was subjected to statistical analysis, as presented in Table 3.1 and 3.2, in terms of median values and standard deviations. Note that the median values were used to reduce the effects of outliers. The refined data was then introduced into the modeling platform (BioWin® and gPROMS). Despite some variation for the wastewater influent concentrations during the monitoring campaign, the concentrations were not measured every day and a dynamic calibration could not be performed based on typical diurnal variations. Instead, the average wastewater influent concentrations were used in the BioWin® and gPROMS and kept constant over the calibration period.

Table 3.1: Summary of plant influent data for model calibration.

| Details | Units | Median | StdDev [%] | Count |
|---|---|---|---|---|
| Influent flowrate | ML/d | 34.8 | 4 | 14 |
| Alkalinity | mg $CaCO_3$/L | 256 | 5.4 | 14 |
| COD | mg/L | 594.5 | 17.9 | 6 |
| TSS | mg/L | 263 | 26.9 | 14 |
| $NH_4^+$-N | mg/L | 38.9 | 11.2 | 14 |
| Total nitrogen | mg/L | 52.8 | 11.8 | 14 |
| $PO_4^{3-}$-P | mg/L | 3.6 | 17.8 | 14 |
| Total phosphorus | mg/L | 7.4 | 14.9 | 14 |

Table 3.2: Summary of plant influent data for model validation.

| Details | Units | Median | StdDev [%] | Count |
|---|---|---|---|---|
| Influent flowrate | ML/d | 30.1 | 40 | 351 |
| Alkalinity | mg $CaCO_3$/L | 248 | 25.9 | 12 |
| COD | mg/L | 584 | 17.6 | 12 |
| TSS | mg/L | 280 | 25.0 | 12 |
| $NH_4^+$-N | mg/L | 38.4 | 13.8 | 12 |
| Total nitrogen | mg/L | 50 | 15.1 | 12 |
| $PO_4^{3-}$-P | mg/L | 4.6 | 31 | 12 |
| Total phosphorus | mg/L | 7.1 | 19.8 | 12 |

### 3.2.3 Plant-wide Model Development

The main modeling platform used to conduct the analysis was BioWin® (`http://envirosim.com/`), and the results have been cross-validated with an implementation of BSM2 in the equation-oriented process simulator gPROMS (`http://www.psenterprise.com/`). BioWin® is routinely used in the wastewater industry as a process analysis tool and to design or upgrade WWTPs. It uses state-of-the-art models of the biological and physical treatment units, and provides support for the adjustment of mode parameters. The model is based on the integrated activated sludge and anaerobic digestion model known as the BioWin® general model developed by Barker and Dold [120]. It has been used for biological nutrient removal, and extended to encompass both the activated sludge and anaerobic digestion models. The biomass separation units consist of three models including point, ideal and flux-based separation models. In this work, the ideal separation model was used throughout the plant because of limited operational data and to reduce numerical difficulties arising from the large number of model variables acting on different time scales from less than a minute to several days as mentioned in the previous Chapter and this would affect the numerical integration. In addition, BioWin® has a new feature to predict direct GHG emissions from biological treatment, especially $N_2O$. $N_2O$ produced by several groups of bacteria involved in nitrification and denitrification. During nitrification $N_2O$ is produced during the oxidation of $NH_4^+$ to $N_2O$ by the AOB, and the production of $N_2O$ is greater at lower concentrations of dissolved oxygen, resulting in the accumulation of $N_2O$. Also, $N_2O$ can be an intermediate product in heterotrophic denitrification, known as incomplete denitrification. Its production is affected by several factors, e.g. the ratio of COD to N, the type of substrate and biomass, pH and temperature. However, to date, there is no indication that nitrite oxidizers (NOB) and anaerobic ammonia oxidiers significantly contribute to $N_2O$ emissions. BioWin® can predict $N_2O$ emissions from the following three mechanisms (Figure 3.2): (i) nitrification by-products whereby part of the

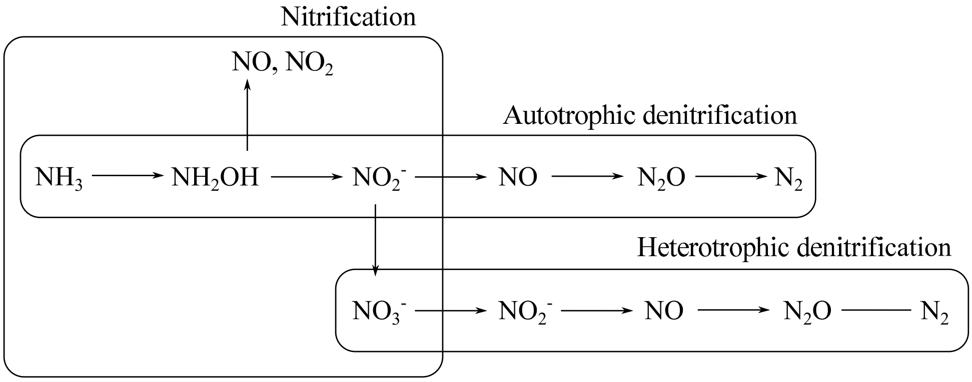



Figure 3.2: $N_2O$ pathway modified from Wrage et al. [163].

ammonia is converted to $N_2O$ by ammonia oxidizing bacteria (AOB) via hydroxylamine oxidation, normally when ammonia is present in excess and without oxygen limitations; (ii) nitrifier denitrification, also mediated by AOBs, but under oxygen-limited conditions, whereby free nitrous oxide (FNA) is used as a terminal electron acceptor to remove nitrite; and, (iii) heterotrophic denitrification, whereby $N_2O$ is produced as an intermediate in denitrification by heterotrophs. Apart from its capability to model effluent quality and fugitive emissions, it is also used to predict aeration energy consumed by activated sludge and aerobic digestion processes here.

Besides BioWin, the plant-wide model was also implemented in gPROMS, which is an equation-oriented process simulator, and features powerful process system analysis and optimisation tools. Here, the unit models in gPROMS were implemented based on ASM2d for the activated sludge process and ideal separation for physical seperation units. Its complementary role, using two modeling platforms, allowed us to cross-compare the simulation results to check consistency. The application of a plant-wide model requires influent fractionation, especially COD and TN, because state variables used in plant-wide models cannot be measured directly, and most measurable variables are based on composite variables. Thus, wastewater fractionation is required so that the model can be used to predict or describe reactions in the system. Additional characterization is required for the calibration step to estimate influent fractionation. Fortunately, BioWin® Influent Specifier developed by EnviroSim Associates Ltd. in an Excel worksheet is used to calculate wastewater influent fractions, and used in both modeling platforms. This worksheet was developed to convert the common measured influent data, e.g. COD, TSS into the variables, e.g. readily biodegradable substrate that can be used in the model, and is based on engineering knowledge and experience. More specifically, the measured components, e.g. COD, TSS, $NH_3$-N, TN were input into the Excel worksheet. Fractions of model components were then adjusted in a given range based on guidelines to match with the measured components. The obtained model components were input into the plant-wide model.

## 3.2.4 Performance Indicators

### 3.2.4.1 Energy Consumption

WWTPs involve many different streams flowing through pipes, and these streams are mostly driven by pumps. In practical terms, the energy used by pumps is the main plant energy demand and accounts for 25 percent of the total energy consumption. The energy consumption of pumps depends on the efficiency of pumps, pipe length, water head, etc., and can be quantified by mathematical expressions; however, most data regarding pumps is not available. One way to track the energy use of pumps is based on the development of regression models which can be based on a simple relationship between power used and stream flowrates through pumps obtained from measurements. Also, energy consumption of pump is practically calculated in combination with process models. Due to the high level of detail in the process models, simplified energy consumption models have been used in many studies [164, 165] and potentially used for the optimisation studies. In this study, the pumps were assumed to operate at a constant efficiency for all flowrates. The historical static energy use, energy break down for each treatment unit, and the flowrate obtained from Sydney Water's energy database were used to develop simple regression models. Then, energy consumption can be expressed as a function of flowrate entering the treatment/separation units. It is worth pointing out that the assumption for calculating energy consumption of pumps is a first/rough approximation and could lead to poor predictions on the cost calculation. Based on the current availability of operational data, the predictions of energy consumption can provide relative trends over different operational strategies. More detail on the pumps, e.g. pump head and pump efficiency which is not currently available can provide more accurate predictions.

Aeration energy in the plant-wide model was calculated based on the mass transfer coefficient, $K_La$, which is related to the superficial gas velocity (the air flowrate per bioreactor cross-sectional area) and diffuser density as follows:

$$K_La = C \cdot U_{SG}^{Y} \tag{3.1}$$

$$C = k_1 \cdot DD^{0.25} + k_2 \tag{3.2}$$

where $k_1, k_2$ and $Y$ are the diffuser parameters specific to the diffuser type. These parameter values are presented in Table 3.3. $DD, U_{SG}$ and $Q_{air}$ represent diffuser coverage, superficial gas velocity, and air flowrate, respectively. The mass transfer coefficient ($K_La$)

Table 3.3: Parameter values for estimating aeration energy in the bioreactor.

| Parameter | Description | Value |
|---|---|---|
| $k_1$ | Correlation parameter | 2.5656 |
| $k_2$ | Correlation parameter | 0.04320 |
| $Y$ | Correlation parameter | 0.82 |
| A | Correlation parameter | -66.7354 |
| B | Correlation parameter | 87.4755 |
| C | Correlation parameter | 24.4526 |

can be used to calculate the aeration energy ($AE$) from the following relationship [164]:

$$AE = \frac{S_O^{sat}}{1.8 \cdot 1000} \sum_{k=1}^{N_{aeration_tank}} V_k \cdot K_La \tag{3.3}$$

where $V$ is the volume of the bioreactor and $S_O^{sat}$ is the saturation concentration of oxygen dependent on temperature which can be calculated as follows:

$$S_O^{sat} = 0.9997743214 \cdot \frac{8}{10.5} \cdot 6791.5 \cdot K \tag{3.4}$$

$$K = 56.12 e^{A + B/T^* + C ln T^*} \tag{3.5}$$

$$T^* = T_K/100 \tag{3.6}$$

where $T_K$ is the temperature of bioreactor in Kelvin.

#### 3.2.4.2 GHG Emissions

Recently, the prediction of GHG emissions from WWTPs has become of great interest to enhance sustainability, and the quantification of GHGs is becoming important to improve insights into carbon flow in WWTPs. Evaluation of GHGs emissions should be accounted for during process design, operation and optimisation of WWTPs [166], and plant-wide mathematical modeling is a promising approach among various alternatives to help improve the understanding of the effects of operational and control strategies on GHG emissions. Also, it can be used to reduce GHG emissions and improve environmental protection. Typically, WWTPs involve three sources of GHG emissions: direct, indirect external and indirect internal [167]. Direct emissions involve biological processes which can be fugitive emissions from biomass respiration; biogas from digesters or gas lines; and indirect external emissions resulting from sources that are not controlled directly in WWTPs e.g. sludge disposal, production of chemicals used in WWTPs. Finally, indirect internal emissions are related to the consumption of acquired or purchased electric/thermal energy. The main GHG emissions from WWTPs include $CO_2$, $CH_4$ and $N_2O$. It is worth noting that $N_2O$ emissions have gained more attention due to its larger global warming potential than $CO_2$ of approximately 298 times [168]. Even low amounts of $N_2O$ emissions could potentially be of concern; thus $N_2O$ emissions were mainly focused in this study. In order to deal with the different elements of GHG emissions, every gas was typically converted into a single unit of $CO_2$ equivalent ($CO_2$e) based on the global warming potential (GWP) over 100 years ($CH_4$ is 25 and $N_2O$ is 298); note that sludge disposal was not considered in this case. The following sources of GHG emissions are included as criteria to evaluate plant performance under different control and operational strategies:

- **Biological treatment** - This is related to the emissions resulting from biological treatment, including biomass respiration and BOD oxidation. This covers GHG emissions during wastewater and sludge treatment generated in the bioreactors and aerobic digesters. Also, $N_2O$ generation as intermediate products from nitrification and denitrification through three pathways is also included in the model prediction, which is available in BioWin®.
- **Overall energy consumption** - This is related to emissions from energy consumption which is mainly from electricity, and involves pumping, mixing and aeration. In this study, there is no energy production from electricity generated by the combined heat and power unit. The conversion factor of energy consumption to GHG emissions used was 0.86 kg $CO_2$/kWh based on electricity purchased from the grid in the local area [169].
- **Chemical usage** - This contribution involved the external carbon source (methanol). Based on the current operation, methanol is added to enhance the denitrification process in Stage 1/2. The conversion factor of chemical usage to GHG emissions is 1.54 g$CO_2$e/g methanol [170].

### 3.2.5 Scenario-based Simulation

A scenario-based approach is applied to quantify the effects of key process variables on WWTP performance, and to identify operational strategies that reduce energy consumption and fugitive emissions at different nutrient discharge levels. These operational improvements were also compared to an alternative plant upgrade scenario based on reverse osmosis to achieve better effluent quality. Different scenarios were selected to show effects of operational strategies which may be carried out by engineers or operators to enhance overall plant performance and/or increase energy efficiency. The following key operating variables were adjusted based on a practical viewpoint and the operating ranges were selected based on guidelines from the real plant to investigate operational strategies to improve the WWTP under study.

- **DO set-point** - It is a key operating variable in the activated sludge process because it has substantial impacts on biological reactions, including biomass growth and sludge settling properties. Also, energy cost from aeration is significantly high, and several studies were carried out to reduce the supplied. It was assumed that the controlller was "perfect" and outputs can reach set-points instantaneously; in this work the DO set-point was varied from 0.2 mg/L to 3 mg/L.

- **Flow splitting** - The WWTP under study was operated with two parallel stages of activated sludge, and the flow splitting process was important because it represents the loads of wastewater to each stage. An overloaded stage can have a detrimental impact on plant performance in terms of effluent quality, energy use and GHG emissions. The flow splitting varied from 35% to 65%.

- **Waste activated sludge** - It is a key operating variable to control SRT or sludge age. SRT is also believed to have an impact on the growth of microorganisms and sludge bulking. In this study, the SRT was varied from 8 to 16 days.

- **Mixed liquor recycle (MLR)** - Activated sludge with predenitrification processes require certain amounts of $NO_3^-$ to be recirculated from aerobic zones where nitrification occurs back to anoxic zones through MLR to combine with organic matter available in wastewater influent for denitrification. Variation of the MLR can greatly affect the level of TN concentration. Note that the oxygen content in the recycle stream may limit the denitrification process.

## 3.3 Results and Discussion

### 3.3.1 Model Calibration

A calibration and first validation was carried out for both the BioWin® and gPROMS models using a combination of routine and non-routine monitoring data. The calibrated models were then used in a scenario-based analysis in order to quantify the links between energy use, effluent quality and fugitive emissions, and to determine improved operational strategies.

In this study, the calibration was conducted to capture the major trends within the plant, with an emphasis on mass conservation and flow splitting. In the first step, the physical separation units consisting of the primary sedimentation tanks, the DAF units, the sludge dewatering units, the tertiary clarifiers and the dual media filters were calibrated based on data from a two-week non-routine monitoring campaign, and validated with 12 months of data (from April 2012-April 2013) from Sydney Water's data management system. Calibration of these physical units was carried out by adjusting either the efficiency of solids removal, or sludge settling parameters as appropriate, so that the predicted liquid and solid outflows would match the available data. The results of the calibration and validation are shown in Figure 3.3 for a primary sedimentation.

Secondly, the bioreactors were calibrated by adjusting a minimal number of kinetic parameters from their default values. Parameter selection for model calibration was based on a sensitivity analysis in order for the predictions to be in good agreement with the primary, secondary, and tertiary effluent concentrations collected during the 2-weeks non-routine monitoring campaign. In this work, local sensitivity analysis was considered based on the steady state simulation relying on the variation of one parameter at a time. First, the simulation was performed based on the default parameter values, then each parameter was varied by a 10% increase/decrease from their default values. The results obtained

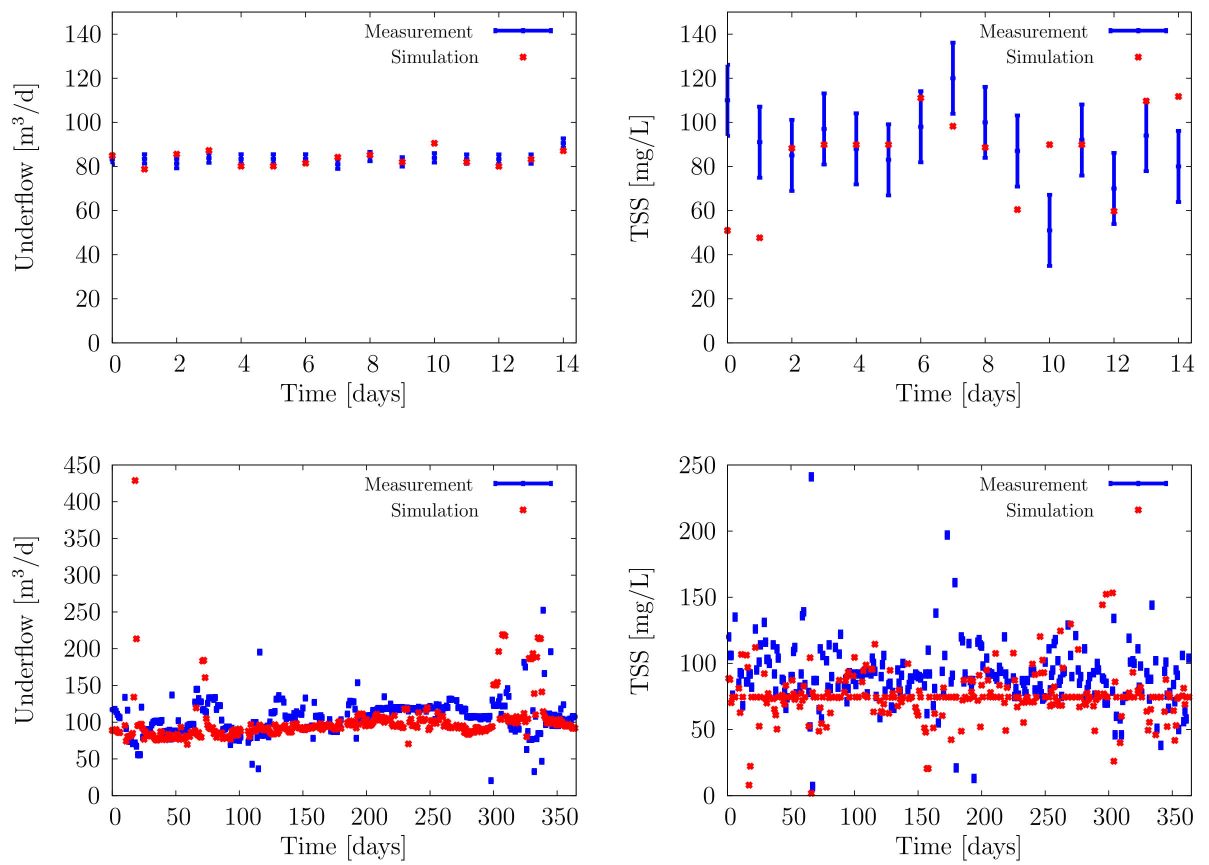



Figure 3.3: Calibration (top plots) and validation (bottom plots) of liquid and solid flows in primary sedimentation tank: underflow, $m^3$/day (left plots) and TSS, mg/L (right plots).

from this sensivity analysis were able to identify the most sensitive parameters in accordance with the model outputs. The results from this sensitivity analysis were later used to prioritize parameters for the model calibration. The adjusted parameters in the BioWin's model corresponded to the nitrite oxidizing biomass (maximum specific growth rate, half-saturation constant for $NO_2$), and the ordinary heterotrophic organisms (fermentation rate) as presented in Table 3.4. Additionally, values of the stoichimetric and kinetic parameters in the gPROMS implementation of the modified BSM2 model have been modified to reflect those used in the BioWin® model. Comparison results reported in Table 3.5 for the tertiary effluent show good agreement between the measured and calibrated values - average values considered here as the variations during the two-week period were small (dry weather). Most of simulated results are within the confidence interval, which means that there is no statistical significant difference for investigated variables between the simulated value and measured data.

Table 3.4: List of kinetic parameters to calibrate the plant-wide model.

| Parameter | Description | Default | Calibration |
|---|---|---|---|
| $\mu_{NOB}$ | Maximum specific growth rate of NOB (1/d) | 0.7 | 0.9 |
| $K_{NO_2}$ | Substrate ($NO_2$) half saturation constant (mgN/L) | 0.1 | 0.25 |
| $q_{fe}$ | Fermentation rate (1/d) | 1.6 | 3.2 |

Table 3.5: Comparison of the predictions with both simulation platforms (after calibration against measurements during the 2 weeks non-routine monitoring campaign for the tertiary effluent (average values).

| | Measurements | Count | BioWin® | gPROMS |
|---|---|---|---|---|
| $NH_4$-N, mg/L | 0.02±0.007 | 14 | 0.08 | 0.09 |
| $NO_3$-N, mg/L | 4.3±0.6 | 14 | 4.4 | 4.8 |
| $PO_4$-P, mg/L | 0.02±0.005 | 14 | 0.04 | 0.04 |
| COD, mg/L | 34±5 | 14 | 31 | 30 |
| MLSS, g/L | 7.7±0.5 | 14 | 7.4 | 7.4 |

In order to validate the plant-wide model, another dataset was used (12 months of data from April 2012 to April 2013). Note that the adjusted parameters from the model calibration were kept constant to obtain matching results. The results of model validation, which are presented in Table 3.6, indicate that there was good agreement between the model predictions and the measured data, although the model was calibrated based on only steady state data. Analysis reveals that the plant-wide model had a predictive ability which was sufficiently accurate for the investigated variables; however, the plant-wide model should be used with caution and engineering judgement. A number of assumptions were made during the investigation due to numerical difficulties in simulating the plant-wide model, and the lack of data availability. It is worth noting that relative trends obtained from the plant-wide model are much more reliable than the absolute performance of model predictions, which makes the plant-wide model well suited for scenario analysis. To improve model calibration and validation, extensive sampling data should be collected including dynamic plant data ranging from less than a minute to several days. In addition, a rigorous model calibration process would be necessary to ensure that the plant-wide model can accurately capture the behavior of the plant.

Table 3.6: Comparison of the predictions with both simulation platforms (after validation against measurements during 12 months of data collection from April 2012 to April 2013 for the tertiary effluent (average values).

| | Measurements | Count | BioWin® | gPROMS |
|---|---|---|---|---|
| CBOD, mg/L | <2 | 84 | <2 | <2 |
| $NH_4$-N, mg/L | 0.02±0.06 | 61 | 0.07 | 0.08 |
| $NO_3$-N, mg/L | 3±0.5 | 61 | 3.4 | 3.7 |
| $PO_4$-P, mg/L | 0.03±0.005 | 60 | 0.03 | 0.04 |
| COD, mg/L | N/A | 0 | 30 | 30 |
| MLSS, mg/L | 7.3±0.15 | 177 | 6.9 | 6.8 |

### 3.3.2 Strategies for Reducing Energy Consumption

Possible strategies for reducing the energy consumption of the plant, without significantly deteriorating the effluent quality or increasing the fugitive emissions (e.g., in the form of $N_2O$). The overall energy consumption in the current plant operation is dominated by compression energy for aeration of the activated sludge tanks in both treatment lines; this high level of aeration results in very low ammonia effluent concentration, less than 0.1 mg/L. This presents a question of whether there could be a better balance between these two parameters. Here, a sensitivity analysis reveals that the dissolved oxygen (DO) set-points in either treatment line and, to a lesser extent, the sludge retention time (SRT) in either treatment line, are most sensitive with respect to the aeration energy among the key operational variables. The effect of various DO set-points (taken as identical in both wastewater and sludge treatment lines) on the energy consumption, ammonia discharge, TN discharge and $N_2O$ emissions is presented in Figure 3.4, showing a tight interplay between these key performance indicators. It is predicted that a decrease in the DO set-point from 2 mg/L to 1 mg/L can decrease the aeration energy by about 15%, with minimal impact on the ammonia discharge, and a reduction in total nitrogen (TN) discharge of 1 mg/L (Figure 3.4a). An extra 10% reduction in aeration energy, and a further 0.5 mg/L reduction in the TN effluent concentration could be achieved when the DO set-point is decreased down to 0.5 mg/L, while the ammonia effluent concentration is kept below 0.2 mg/L. In contrast, the low DO set-point can have a negative impact on global climate change because decreasing the DO set-point leads to an increase in the

$N_2O$ emissions due to incomplete nitrification, which increases by a factor of 3 between 0.5 mg/L and 2 mg/L (Figure 3.4b). It is also interesting to note that operating at the low DO set-point may also have other adverse effects on the treatment quality, such as poor sludge settleability, which is not considered in the model.

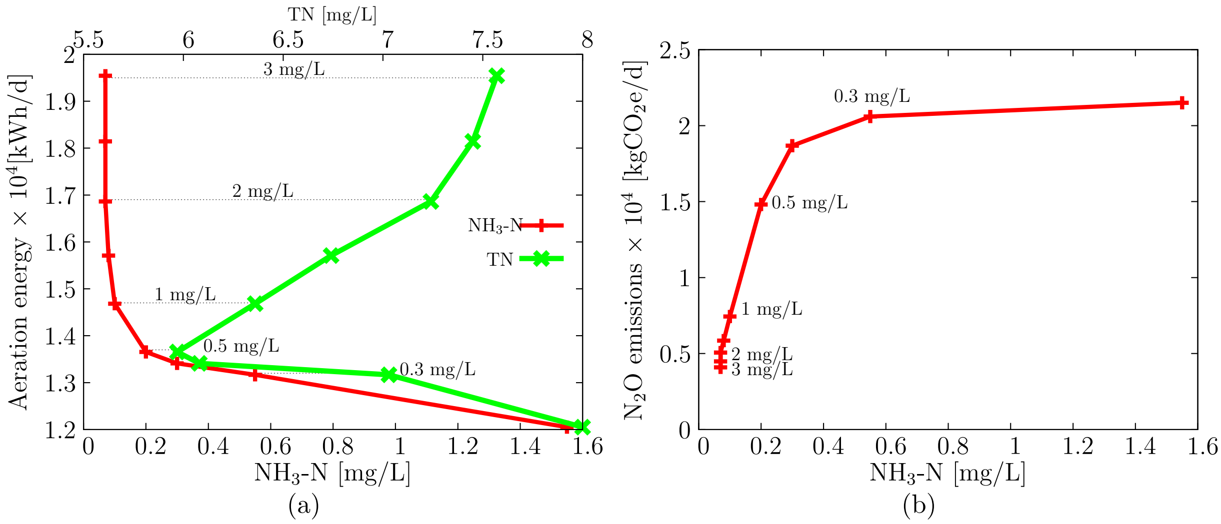



Figure 3.4: Effect of DO set-points on (a) the aeration energy, effluent quality ($NH_3$-N represented by the red line and TN represented by the green line) and (b) $N_2O$ emissions (The concentrations in Figure (3 mg/L, 2 mg/L, 1 mg/L, 0.5 mg/L and 0.3 mg/L) indicate the DO-setpoints).

Other studies have also investigated the general trends in energy consumption and fugitive emissions when the DO set-point is varied, and a comparison between our results and those reported by Flores-Alsina et al. [138] is presented in Table 3.7. Note that the overall GHG emission values at different DO set-points are consistent, and show a similar trend for lower DO set-points. Although off-site $CO_2$ emissions may decrease, this effect is counterbalanced by increased $N_2O$ emissions, especially since $N_2O$ has a 300-fold stronger greenhouse effect than $CO_2$. In addition, our modeled $N_2O$ emissions are between 0.009 and 0.027 kg$N_2O$ per kg N in the influent. This is in the medium range compared to other full-scale WWTPs, typically between 0.001 and 0.25 kg$N_2O$/kg N influent, which vary widely depending on a plant's configuration or operation [171, 172]. Similarly, the effect of SRT variation in Stage 1/2 (keeping the SRT in Stage 3 at its current nominal value) on the energy consumption, TN discharge and $N_2O$ emissions (shown in Figure 3.5) was also investigated. It is noted that the effect of varying the SRT in Stage 3 had similar

Table 3.7: Comparison of the overall GHG emissions at various DO set-points with those from the work by Flores-Alsina et al. [138] - the reported values are per $m^3$ of treated wastewater.

| DO set-point | This work | Flores-Alsina et al. [138] |
|---|---|---|
| 0.5 mg/L | 1.19 $kgCO_2e/m^3$ | N/A |
| 1 mg/L | 1.02 $kgCO_2e/m^3$ | ca. 1.6 $kgCO_2e/m^3$ |
| 2 mg/L | 1.00 $kgCO_2e/m^3$ | ca. 1.25 $kgCO_2e/m^3$ |
| 3 mg/L | 1.04 $kgCO_2e/m^3$ | ca. 1.3 $kgCO_2e/m^3$ |

results. It is possible to reduce the aeration energy by a small percentage by decreasing the SRT (Figure 3.5a), and therefore the extent of endogenous decay, but this then leads to increasing the energy/cost of sludge treatment at the same time. A reduction in the SRT is also accompanied by an increase in $N_2O$ emissions (Figure 3.5b), although, again, this is small compared to GHG emissions from the related energy use. Regarding the effluent quality, Figure 3.5 shows that the effect of reducing the SRT would be beneficial in terms of the TN concentration, with possible reductions over 1 mg/L. This is mainly due to a reduction in nitrate concentration, whereas the ammonia concentration remains below 0.2 mg/L despite a decrease in the nitrifier biomass for lower SRT values.

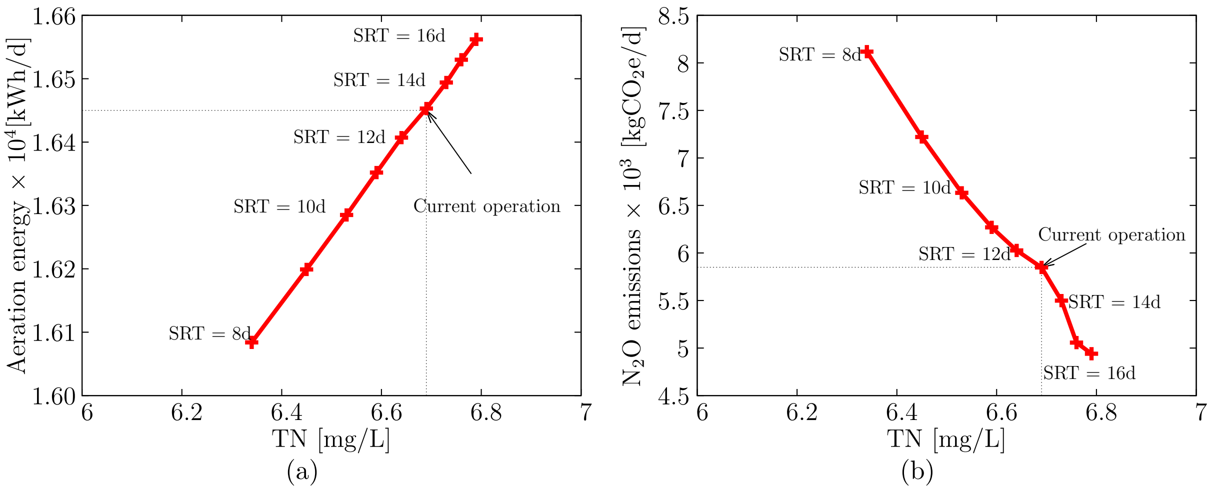



Figure 3.5: Effect of SRT in Stage 1/2 on (a) the aeration energy, effluent quality and (b) $N_2O$ emissions.

On the whole, decreasing the DO set-points and the SRT could lead to a significant reduction in energy consumption and a lower TN effluent concentration, while maintaining a very high treatment quality regarding ammonia and keeping $N_2O$ emissions at an acceptable level compared to other GHG emissions. It is pointed out that $NH_3$-N and TN that are not removed in the plant can be released to the environment. This can be an important source of $N_2O$ emissions in the river up to 0.68 Tg/yr of anthropogenic N inputs estimated by the river network models [173] so further study on incorporation of GHG emissions from river or water receiving body should provide more picture of the overall GHG emissions. Regarding the characterization factors (GWP100) used to combine the environmental impact of $N_2O$ and $CH_4$ with other environmental impacts including energy consumption, these values have been used by several studies [138, 174]. Even though these values are relatively high, an increase or decrease (10%) from the default values would slightly affect the overall GHG emissions (less than 5%). This is because direct emissions, e.g. $N_2O$ and $CH_4$ are only one part of GHG emissions and the main contribution of the overall GHG emissions is from energy consumption.

### 3.3.3 Strategies for Enhanced Nutrient Removal

Strategies for improving the effluent quality are also investigated, without causing a large increase in energy consumption or fugitive emissions. Given that the plant already achieves low ammonia and phosphate discharge, the analysis has focused on enhancing nitrate removal. The major bottleneck in the current operation appears to be low carbon availability for denitrification in the anoxic tanks of both treatment lines. Especially sensitive in this context are the operational variables corresponding to the influent flow split between Stage 1/2 and Stage 3, and the mixed-liquor recirculation (MLR) rate.

The effect of varying the influent fraction between Stage 1/2 and Stage 3 was investigated ranging from 35% to 65% (current operation 46%), and the corresponding trends are shown in Figure 3.6. Increasing the influent fraction to Stage 1/2 results in a possible reduction of the TN effluent concentration by about 1 mg/L (Figure 3.6a). Further inspection reveals that the TN concentration in the Stage 1/2 effluent is at a minimum for a split fraction of around 55% (compromise between a sufficient residence time in the anoxic tanks and the need for a high enough C:N ratio). Whereas, the TN concentration in the Stage 3 effluent is decreased with increasing influent flow to Stage 1/2. It is noted that there is a limited effect of the influent flow splitting on the aeration energy or the final ammonia effluent concentration, which remains below 0.2 mg/L for influent fraction in the range of 35-65%. For the $N_2O$ emissions, they are predicted to increase as a larger fraction of the wastewater is treated in Stage 1/2 (Figure 3.6b) due to incomplete nitrification, which leads to nitrite accumulation in the anoxic tank of Stage 1/2 despite a decrease in these emissions in Stage 3. It was also observed that the small amount of methane emissions from the anaerobic reactor in Stage 3 slightly increased. However, all these fugitive emissions remain small compared to energy-related GHG emissions.

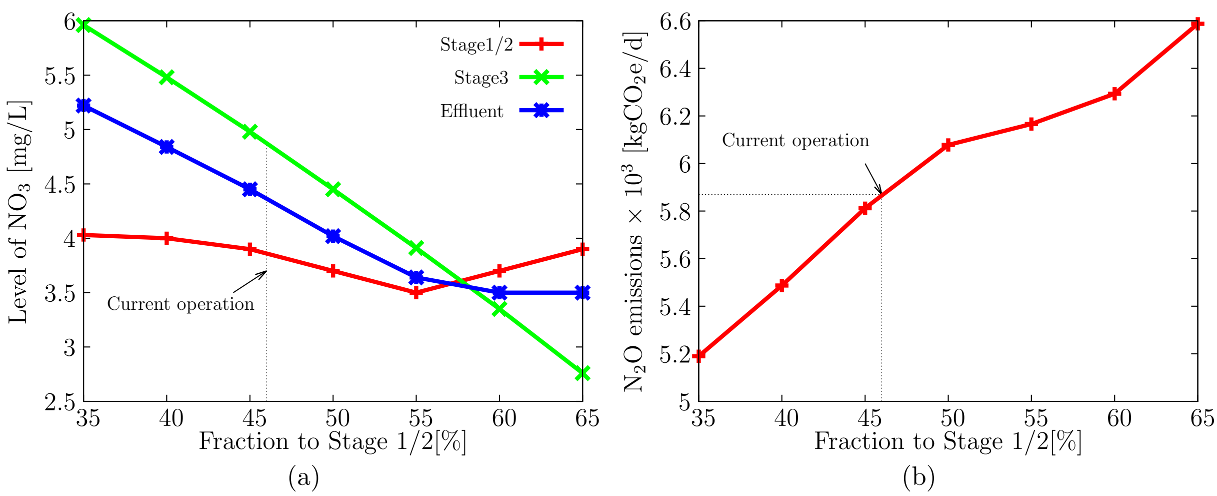



Figure 3.6: Effect of influent split between Stage 1/2 and Stage 3 on (a) the $NO_3^-$ discharge and (b) $N_2O$ emissions.

As expected, an increase in the MLR in either treatment line can lead to sending around a larger amount of $NO_3^-$ back to the anoxic zone where denitrification occurs and, as a result, a reduction in the $NO_3^-$ effluent concentration is predicted. For the Stage 1/2, the effect of MLR variation is illustrated in Figure 3.7a, showing a potentially significant decrease in $NO_3^-$ concentration; it is noted that similar behaviour is observed with Stage 3; typically, such a reduction would entail larger pumping energy/costs. With regard to $N_2O$ emissions, greater emissions are predicted when increasing the MLR in Stage 1/2 (Figure 3.7b); this is possibly because a large MLR can result in an excessively low C:N ratio, which then leads to nitrite accumulation. On the other hand, an increase in the MLR in Stage 3 can result in a reduction in the $N_2O$ emissions because the C:N ratio is not limited in this stage of treatment.

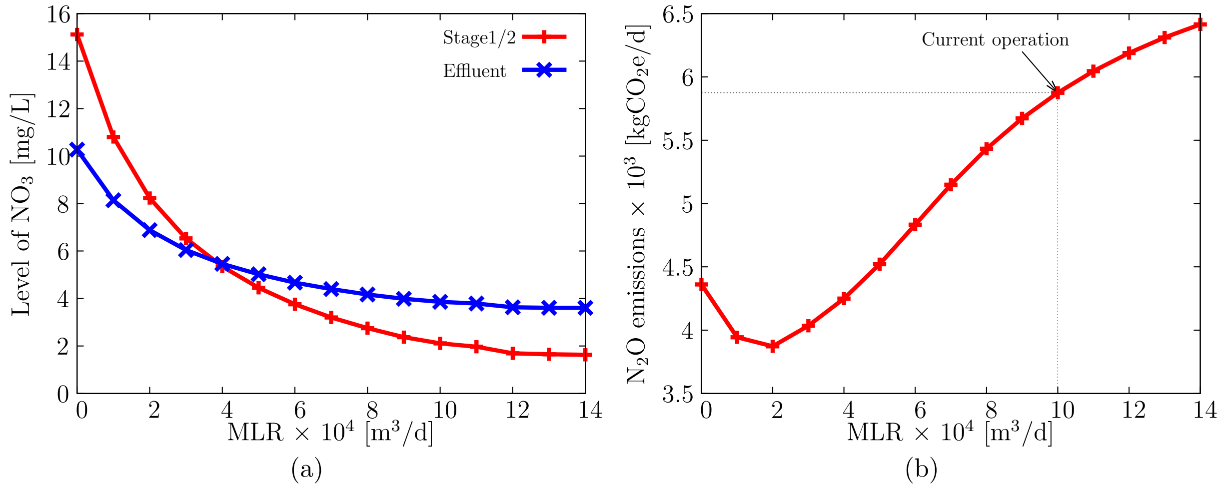



Figure 3.7: Effect of varing mixed-liquor recycling (MLR) in Stage 1/2 on (a) the $NO_3^-$ discharge and (b) $N_2O$ emissions.

By and large, this analysis suggests that increasing the influent split to Stage 1/2 as well as increasing the MLR in both stages could lead to a lowering of the TN discharge concentration to approximately 3 mg/L, while not causing a large increase in aeration energy and keeping fugitive emissions at a low level compared to other GHG emissions.

In the near future, the EPA licenses on effluent quality are likely to be stricter. The low concentrations of nutrients are required at this WWTP to reduce the nutrient load to the river which is sensitive to the algae bloom. A new way to treat wastewater will be used to provide the better effluent quality. The alternative way to enhance nutrient removal is to use reverse osmosis (RO). The RO was already installed at the WWTP to recycle water that can be used in many ways. The volume of nutrients is reduced to provide high quality similar to drinking water as the key part of the plan to increase water recycling. Membrane technology might become necessary to achieve the required level of effluent quality with stricter effluent quality regulations, or in cases of wastewater reclamation. Currently, a fraction of the wastewater from the WWTP is being polished in an advance process where RO is used; after RO the TN concentration in the effluent could be as low as 0.3 mg/L. This scenario was compared with the other three scenarios evaluated in terms of energy use and GHG emissions from the modelled treatment plant with TN discharge concentrations of 3 mg/L, 5 mg/L and 8 mg/L. The results of all these scenarios are presented in Figure 3.8, with their respective energy consumption and $CO_2$-equivalent emissions [175, 176]. It can be seen that advanced treatment (RO) would contribute to substantial increases in energy consumption and GHG emissions by about 50% in comparision with those scenarios in which RO is not included, and this would have an increased negative impact on the environment. Hence, this scenario-based modeling provides a means of incorporating a broader picture of the environmental benefits and drawbacks of upgrading to RO.

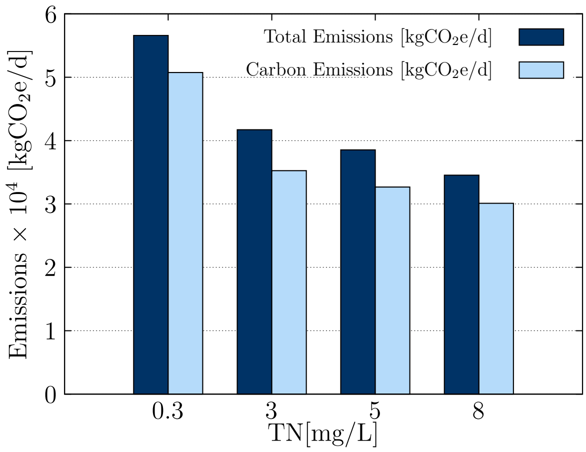



Figure 3.8: Comparison of plant upgrade scenarios, including operational changes and reverse osmosis, in terms of TN discharge and GHG emissions (both fugitive and energy related).

## 3.4 Summary

This chapter has presented the application of a plantwide model-based methodology to conduct a detailed analysis of operational strategies on energy use, effluent quality and fugitive emissions for an existing WWTP which operates two parallel treatment stages. The key improvemence and difference from other similar studies is that the plant-wide model under study is able to identify what level of nutrient discharges, energy consumption and GHG emissions can be reduced and what impact of further reduction in nutrient discharges has on the overall plant performance. This is important information used to identify the main trade-off between effluent quality, energy consumption and GHG emissions. Also, this study presents the model calibration to the full-scale WWTP based on routine and non-routine measurements. Quantitatively, potential improvements have been identified by the plant-wide model to reduce energy consumption. It is suggested that the energy consumption could be reduced by up to 10-20% by manipulating the DO set-point and SRT based on the nominal condition in both treatment stages. However, these changes can typically lead to an increase in $N_2O$ emissions because of incomplete nitrification or denitrification. In addition to potential improvements to reduce the energy consumption, a scenario-based analysis was conducted to identify potential improvements to decrease nutrient discharge. It was found that the nitrate concentration in the tertiary effluent could potentially be reduced to approximately 3 mg/L through operational changes to the influent splitter fraction between treatment stages, and the MLR rate in both stages. As the licenses on effluent quality is likely to be stricter in the near future, an alternative way to treat wastewater is implemented to provide better effluent quality before discharge water into the river where is particular sensitive to the algae bloom. Further improvement of effluent quality can be performed through RO installed at the current WWTP to recycle water. The RO can treat water to reach the high level of quality similar to potable water. Expectedly, RO could potentially enhance nutrient removal down to 0.3 mg/L, but this would entail an energetic penalty with a corresponding increase in GHG emissions of up to 50%. Such a model-based methodology provides valuable information about the impact of wastewater treatment on the environment and could be used to guide discussions about environmental licensing of existing WWTPs.

# Chapter 4

# Plant-wide Model-based Optimisation of WWTP Operation

## 4.1 Introduction

WWTPs involve a number of processes to remove organic matter and nutrients such as activated sludge and/or anaerobic digestion. Operation of WWTPs is another important aspect to consider to improve the performance of WWTPs in terms of effluent quality and energy use. Descoins et al. [143] stated that researchers in the wastewater community have mainly focused on modeling and associated water quality. More effort should focus on the link between water quality, the removal efficiency of WWTP contaminants, and energy aspects because energy is inextricably interconnected with economic and environmental issues. Plant-wide models and rigorous optimisation techniques can be useful for this problem because they allow us to capture the overall performance of each treatment/separation unit, and provide a better understanding of the biological and physical mechanisms, including their interactions. In this chapter, a plant-wide model-based optimisation is applied to another activated sludge plant with anaerobic sludge treatment, owned and operated by Sydney Water. The aim is to; (i) quantify the impacts of key operating variables on effluent quality and energy use to develop a better understanding of what level of nutrient discharges can be reduced without a significant increase in energy consumption, (ii) develop optimised operational strategies to enable plant managers to trade-off these conflicting objectives, and (iii) incorporate uncertainty into a plant-wide model to increase the robustness of plant-wide model predictions through the application of robust optimisation methods. The Chapter is organised as follows: Section 4.2 is concerned with plant-wide model development, and presents the calibration/validation of this model based on existing plant-data. Then, Section 4.3 describes the scenario-based optimisation approach and discusses the results in light of the aforementioned objectives.

## 4.2 Plant-wide Model Development

### 4.2.1 Plant Description

The WWTP under study is a tertiary plant owned and operated by Sydney Water, which is designed to treat a population load of 210,000 population-equivalents, and the treated effluent is discharged into coastal waters. The layout of this plant is shown in Figure 4.1; the wastewater influent initially undergoes screening and primary sedimentation to remove large particulates. Then, the wastewater is sent to secondary treatment, consisting of five parallel aerobic/anoxic tanks (modified Ludzack-Ettinger process) for carbon and nitrogen removal. The wastewater is finally polished by sand filtration and UV disinfection before being discharged to the coastal waters. The UV disinfection was not included in the model configuration because it does not affect the selected/monitored effluent quality, e.g. COD, TKN, or nitrate. In addition to the wastewater stream, sludge produced in primary and secondary treatment are mixed, thickened and digested anaerobically before disposal. It is noteworthy that the quality of the treated effluent is usually better than the required standards, especially with regards to ammonia discharge to maintain suitable effluent quality even when unpredictable situations. This WWTP is flexible enough for exploration of a wide range of scenarios, and it presents excellent potential for optimisation due to substantial interactions between different liquid and sludge treatment stages.

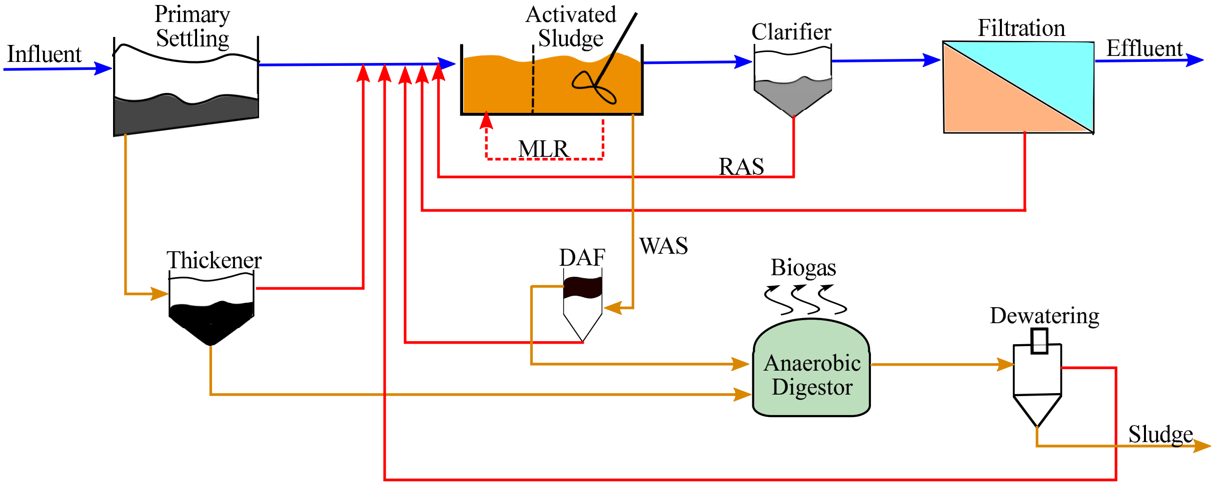



Figure 4.1: Layout of the activated sludge plant with anaerobic digestion treatment.

### 4.2.2 Plant-wide Model Formulation

This subsection presents the main components of plant-wide model, which is based on the interface approach (see Section 2.5.1.3) and the benchmark model BSM2. The latter is commonly used for assessing process performance, control system evaluation, etc [116], and is available in several commercial wastewater treatment process simulators, including GPS-X®, SIMBA® and WEST®. The general layout of BSM2, which is shown in Figure 4.2, is indeed very similar to the actual plant under consideration in Figure 4.1. A brief description of the main units and interfaces is given in the following subsections.

#### 4.2.2.1 Activated Sludge Model

The activated sludge process is the most commonly used biological treatment in WWTPs. Several models for the activated sludge process have been developed to describe the process, especially models from the ASM family (ASM1, ASM2, ASM2d, ASM3) proposed by the International Water Association (IWA) [110]. They are increasingly dominant and represent a major contribution to the wastewater treatment community. Also, these are considered as state-of-the-art models of the activated sludge process, and are used in most commercial process simulators. For BSM2, ASM1 is selected to describe the biological reactions of carbon and nitrogen in the bioreactor as depicted in Figure 4.3. The model

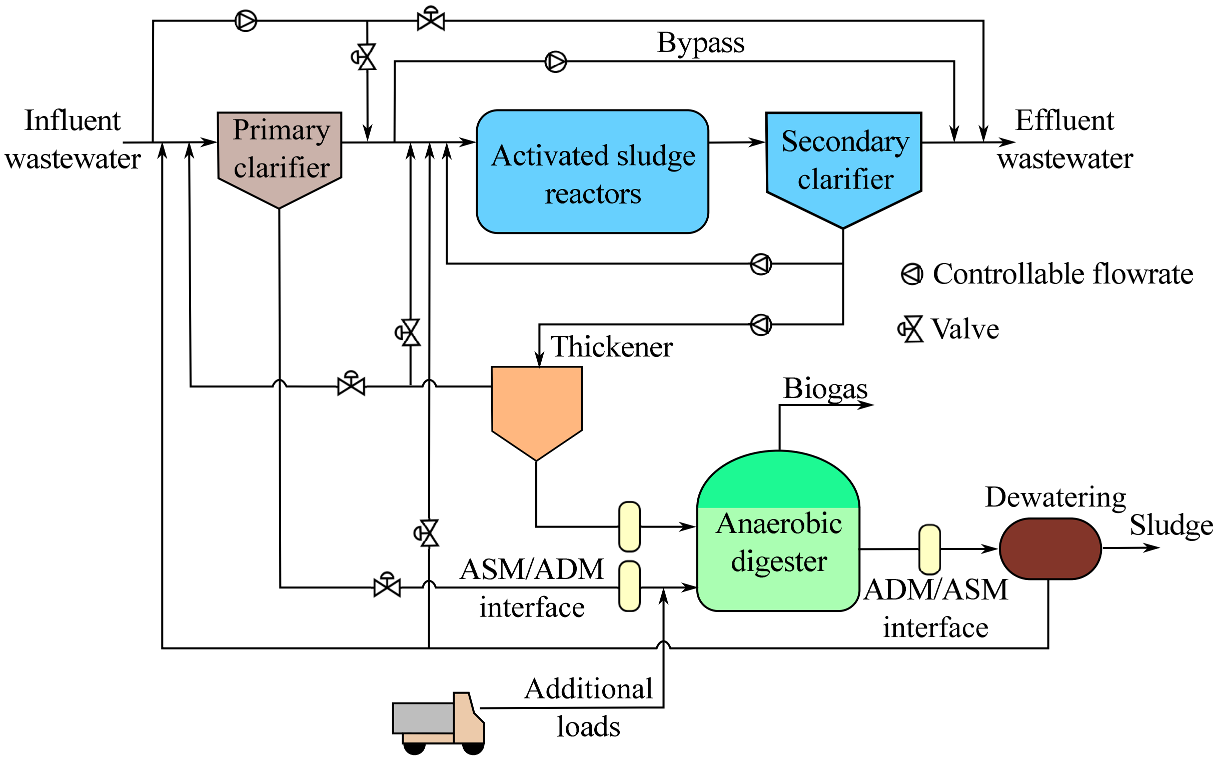



Figure 4.2: Plant layout for the BSM2 modified from Jeppsson et al. [116].

consists of 13 variables and eight processes to describe biological behavior, and use Monod kinetics to describe the biological growth rates of these processes. Further details of ASM1 is available in Henze et al. [111].

#### 4.2.2.2 Secondary Sedimentation

Secondary sedimentation is the unit operation where biomass and other solids settle out from the clear treated effluent after biological treatment. A certain fraction of the sludge is sent back to combine with inlet streams to maintain a good population of biomass in the bioreactor, while the remaining sludge undergoes treatment. The settling model developed by Takács et al. [177] is commonly used, and is modeled as a multi-layer non-reactive model based on the solid flux and mass balance around each layer and uses a double exponential settling function to describe the settling velocity on the sludge concentration. Note that gravity settling is calculated by the solid flux–the product of the settling velocity and the solid concentration in each layer. More detail of the sedimentation model is available in several technical reports and in the published literature [165, 177].

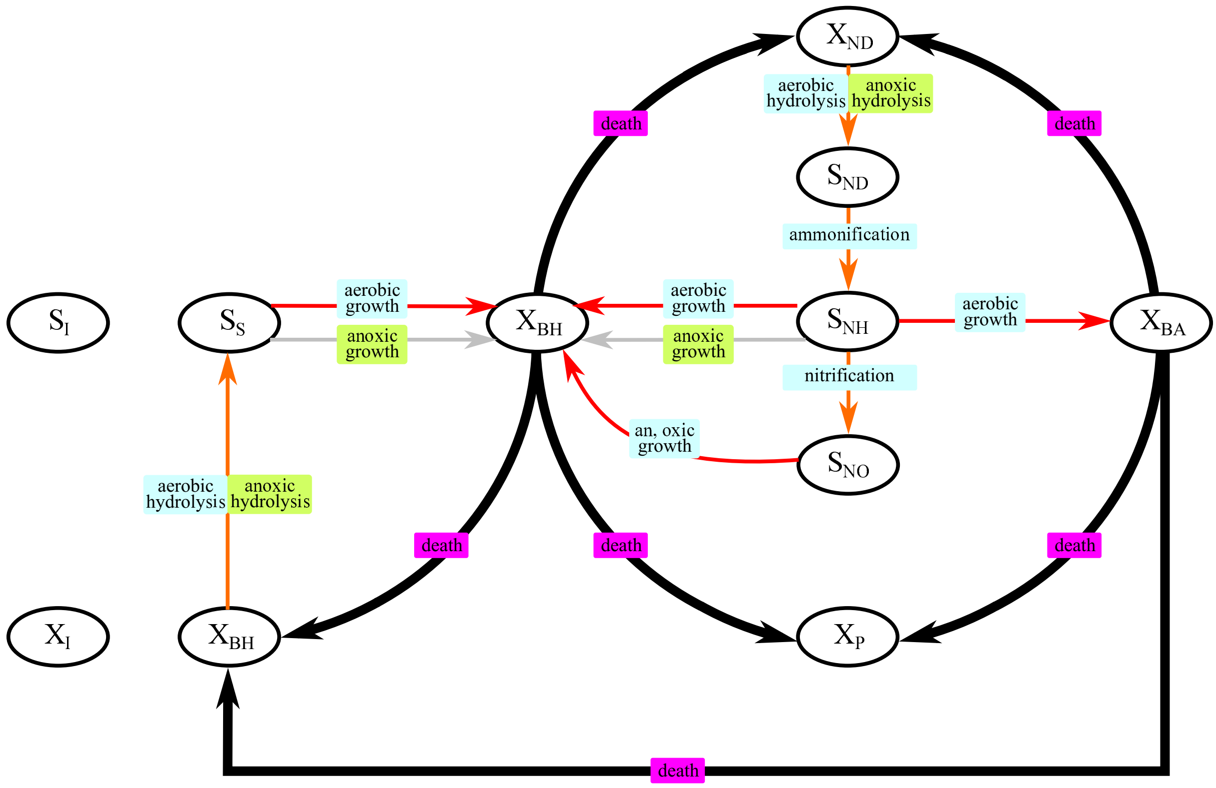



Figure 4.3: Schematic representation of ASM1 modified from Alex et al. [165].

#### 4.2.2.3 Anaerobic Digestion Model

The Anaerobic Digestion Model No. 1 (ADM1) developed by Batstone et al. [114] is widely recognized and used for modeling the anaerobic digestion process,and has been implemented and validated in several software platforms. The model considers biological reactions in the liquid and gas phases, including gas- liquid interactions. The ADM1 for the plant-wide model was modified from its orginal version in terms of inhibition functions, gas flow calculations etc., because of computational difficulties (the model is stiff because the range of time scale is large from a second to months), and no explicit values being available for carbon and nitrogen contents for some state variables in Batstone et al. [114]. Note that the model variables used are different from other models so a model interface is needed. More details of the ADM1 model for the platform-wide implementation are available in Rosén et al. [178].

#### 4.2.2.4 Primary Sedimentation Model

The primary sedimentation model is based on Otterpohl and Freund [179], and Otterpohl et al. [180]. The model assumes no biological activity in the settler, which is described as a completely mixed tank. Effluent is divided into water and sludge streams based on an empirical expression which considers hydraulic retention time, and the ratio of particulate to total COD. Soluble components are assumed to be not affected and equal to the inlet for both outlet streams. The flowrate of sludge is set to be proportional to the influent flowrate; more detail of the primary sedimentation model is available at Otterpohl and Freund [179] and Otterpohl et al. [180].

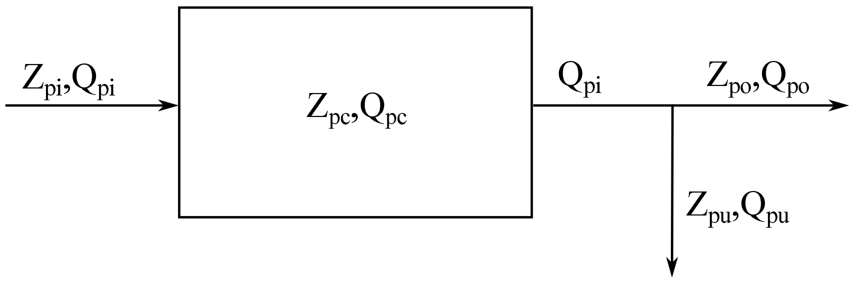


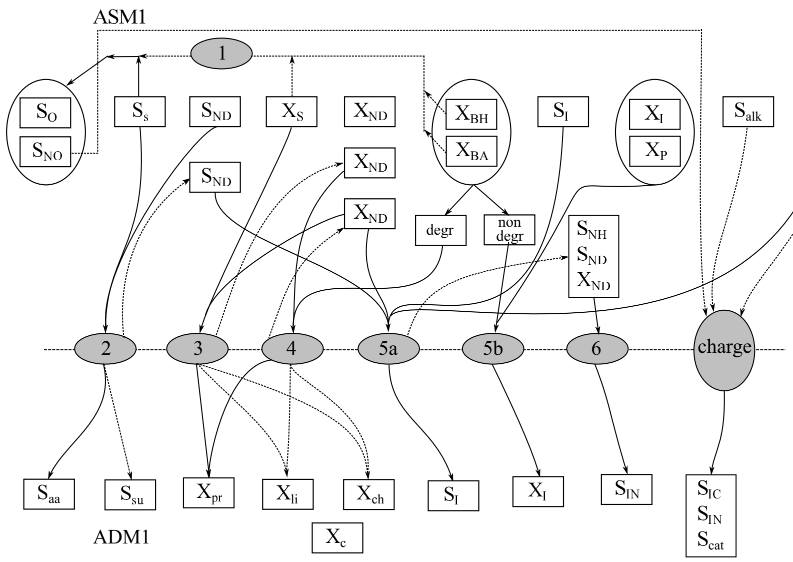

Figure 4.4: Schematic representation of proposed primary sedimentation model modified from Otterpohl and Freund [179] and Otterpohl et al. [180].

#### 4.2.2.5 Thickener Model

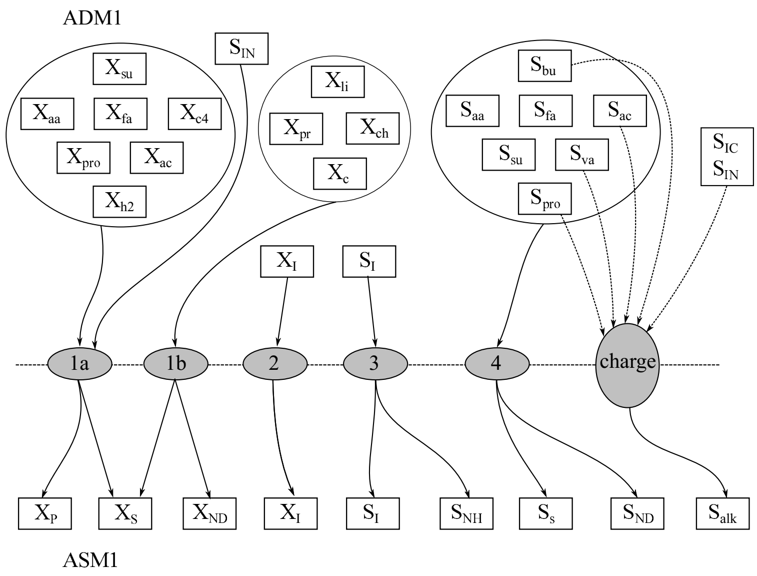
For simplification, the thickener, filtration and dewatering units are modeled as ideal and continuous processes without biological reaction. Most particulate matter fed into the thickener or dewatering units is assumed to be settled and discharged in the sludge stream. The model does not consider the change of sludge characteristics and assume good settling qualities. Concentrations of soluble components are equal in both outlet streams which are identical to the inlet concentrations.

#### 4.2.2.6 Interface Model

Variables in the activated sludge and anaerobic digestion models are different, so a model interface is necessary to combine the two process variables, and researchers in the wastewater treatment community have developed a number of interface models. The ASM1/ADM1 interface, developed by Nopen et al. [122], is a promising version among the various alternatives, and has been used along with the BSM2 in several applications; it is modified from the model interface developed by Copp et al. [123]. The ASM1/ADM1 interface initially removes oxygen and $NO_3^-$-N in wastewater with a reduction in associated COD. The remaining COD and nitrogen are converted directly into proteins, lipids, carbohydrates, inerts, amino acids and sugars based on corresponding nitrogen fractions, and soluble and particulate fractions. In the final step, the inorganic fractions are calculated to balance the charge interface, as shown in Figure 4.4a. For the ADM1/ASM1 interface, the concept is similar to the ASM1/ADM1 interface, which maps the biomass, COD and nitrogen variables of ADM1 into ASM1 variables directly based on corresponding fractions of nitrogen. Finally, the charge is calculated to balance alkalinity (Figure 4.4b).




(a)




(b)

Figure 4.4: Schematic representation of the interface model modified from Nopen et al.[122].

### 4.2.3 Calibration Procedure and Results

Model calibration of the WWTP under study is based on historical plant data for a 6-month period, obtained from Sydney Water's data management system. Historical data is routinely collected from online measurements and from laboratory analysis. The laboratory analysis is performed both onsite at the WWTP, and at a laboratory accredited by the Australian National Association of Testing Authorities. The data set consists of the wastewater average daily flow, solids flows and concentrations to and from the main separation units, MLSS concentration in the aeration tanks, effluent concentrations, and the biogas production. Additionally, measurements of the wastewater composition are available (from September to March), as reported in Table 4.1 in terms of their mean values and standard deviations. Given the rather large uncertainty regarding the wastewater composition for the calibration data set, a two-step calibration procedure is used in order to capture the main trends in the plant, focusing primarily on mass conservation and flow splitting [152, 181]. The first step involves calibration of the physical separation unit models, including the primary sedimentation tanks, thickener units, dissolved-air flotation (DAF) units, secondary clarifiers, and tertiary filters. Specifically, adjusting the solids removal efficiency or other sludge settling parameters as appropriate is carried out,

Table 4.1: Summary of plant influent data for model calibration.

| Details | Units | Median | StdDev [%] | Count |
|---|---|---|---|---|
| Alkalinity | mg $CaCO_3$/L | 231.0 | 14.6 | 6 |
| COD | mg/L | 569.0 | 40 | 6 |
| TSS | mg/L | 296.0 | 24 | 18 |
| $NH_4^+$-N | mg/L | 42.9 | 26 | 6 |
| Total nitrogen | mg/L | 61.3 | 24 | 6 |

in order for the predicted flows and solids concentrations to match the available data in the least-squares sense. The calibration results are shown on Figure 4.5, and the corresponding calibrated parameters for each unit are reported in Table 4.2. The calibrated flows and solids concentrations are found to be in good agreement with the corresponding measurements for all the separation units. Besides the use of simple separation models (static input-output maps), and the fact that a single parameter is adjusted for each one of them, the observed mismatch between the predictions and measurements from one day to the next can also be attributed to the use of daily averages for the flows and concentrations. Note that the main objective in this study is to capture the major trends of the plant-wide behavior which is well-predicted by the model predictions. However, the current accuracy is limited by the availability of operational data. In order to improve the accuracy of model predictions, more consistently operational data, e.g. TSS and data from experimental design is needed, e.g. sludge volume index (SVI).

Table 4.2: Calibrated model parameters in separation units.

| Unit | Parameter | Value |
|---|---|---|
| Primary settling | $f_{corr}$ (Correction factor) | 0.61 |
| Clarifier | $f_{ns}$ (Non-settleable fraction) | 0.01 |
| DAF | $\eta_{TSS}$ (TSS removal efficiency) | 0.99 |
| Thickener | $\eta_{TSS}$ (TSS removal efficiency) | 0.98 |
| Filter | $\eta_{TSS}$ (TSS removal efficiency) | 0.94 |
| Dewatering | $\eta_{TSS}$ (TSS removal efficiency) | 0.98 |

The second step involves calibration of the biological processes in the plant-wide model, as described by ASM1 and ADM1, for the aerobic/anoxic tanks and the anaerobic digesters, respectively. The idea is to adjust selected parameters in order for the predicted

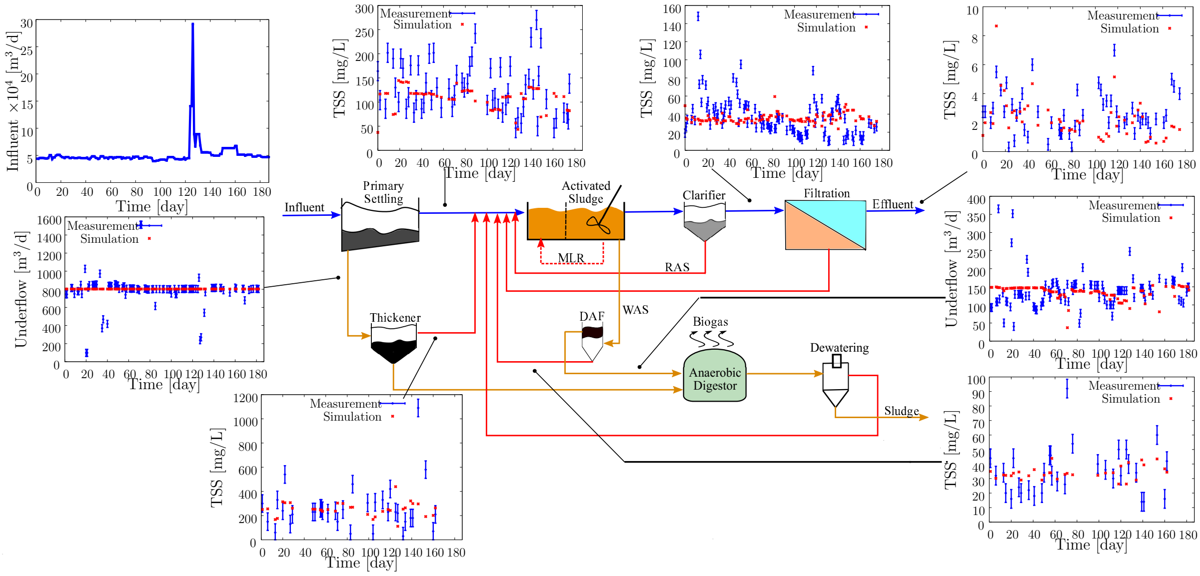



Figure 4.5: Calibration of liquid and solid flows in the physical separation units.

MLSS, effluent concentrations, and biogas production to match their corresponding measured vlaues. Given the rather large uncertainty on wastewater composition (see Table 4.1), the focus here is on adjusting the influent fractions, while keeping the kinetic and stoichiometric parameters in ASM1/ADM1 at their default values. Although fine-tuning certain kinetic or stoichiometric parameters can help further close the gap between predictions and measurements, it is found that the resulting estimates fail to be statistically meaningful given the lack of plant data here, which could be detrimental to the prediction capability (robustness) of the model. Fractionation of the influent in BSM2 is based on the state variables in ASM1 [111, 116]. Apart from the inlet concentrations of ammonia and alkalinity whose values can be directly determined from the influent measurements, it was assumed as a first approximation that no heterotrophic biomass, autotrophic biomass, products of biomass decay, or nitrate are brought in with the influent. This leaves us with the following six influent fractions to determine: inert soluble organic matter ($f_{S_I}$); readily biodegradable substrate ($f_{S_S}$); inert particulate organic matter ($f_{X_I}$); slowly biodegradable substrate ($f_{X_S}$); soluble biodegradable organic nitrogen ($f_{S_{ND}}$), and; slowly biodegradable organic nitrogen ($f_{X_{ND}}$). Moreover, these fractions must satisfy the following relationships.

$$f_{S_I} + f_{S_S} + f_{X_I} + f_{X_S} = 1 \tag{4.1}$$

$$0.75(f_{X_I} + f_{X_S}) = 1 \tag{4.2}$$

$$f_{S_{ND}} + f_{X_{ND}} + 0.06\frac{COD}{TN} f_{X_I} + \frac{NH_4^+ - N}{TN} = 1 \tag{4.3}$$

When inlet concentrations of COD, TSS, TN and $NH_4^+$-N are specified, the influent fractionation problem thus has 3 degrees of freedom only. The fractionation results obtained by considering the mean influent concentrations in Table 4.1, together with default kinetic/stoichiometric parameters in ASM1 and ADM1, are reported in the Set #1 column in Table 4.3; the corresponding model predictions are shown in Figure 4.6 (red line). A good agreement is observed overall between the model predictions and the measurements during the 6 month period. The main trends appear to be captured well by the plant-wide model, with the exception of biogas production whose rate is underestimated by 25-30% during the first 120 days. Nonetheless, the fact that the predicted MLSS concentration in the aeration tank follows the measurements well during the same period indicates that such a discrepancy could be due to the mean COD and/or TSS influent concentrations in Table 4.1 being underestimated themselves. To confirm it, both influent COD and TSS concentrations have been estimated along with their fractionation in a separate calibration. These results are reported in the Set #2 column in Table 4.3, with the corresponding model predictions also shown on Figure 4.6 (green line). The optimised COD and TSS inlet concentrations are expectedly larger than the mean values used in initial calibration, yet within the standard deviation range of Table 4.3, thereby leading to a reduction in the biogas production rate mismatch. Both calibration sets are considered subsequently for the plant-wide analysis and optimisation. Because the plant-wide model with default kinetic and stoichiometric parameters may provide limited predictive capability for certain key process variables, such as biogas production, a similar calibration procedure for another data set was conducted. The fractionation results obtained by considering the mean influent concentration in Table 4.4, are presented in the Set #1 column in Table

Table 4.3: Calibrated parameters of the wastewater influent and its fractionation.

| Parameter | Unit | Set #1 | Set #2 |
|---|---|---|---|
| $f_{\mathrm{SI}}$ | g(COD)/g(COD) | 0.06 | 0.05 |
| $f_{\mathrm{SS}}$ | g(COD)/g(COD) | 0.25 | 0.16 |
| $f_{\mathrm{XI}}$ | g(COD)/g(COD) | 0.07 | 0.07 |
| $f_{\mathrm{XS}}$ | g(COD)/g(COD) | 0.62 | 0.72 |
| $f_{\mathrm{SND}}$ | g(N)/g(N) | 0.16 | 0.11 |
| $f_{\mathrm{XND}}$ | g(N)/g(N) | 0.10 | 0.15 |
| COD | mg/L | 569 | 597 |
| TSS | mg/L | 296 | 350 |

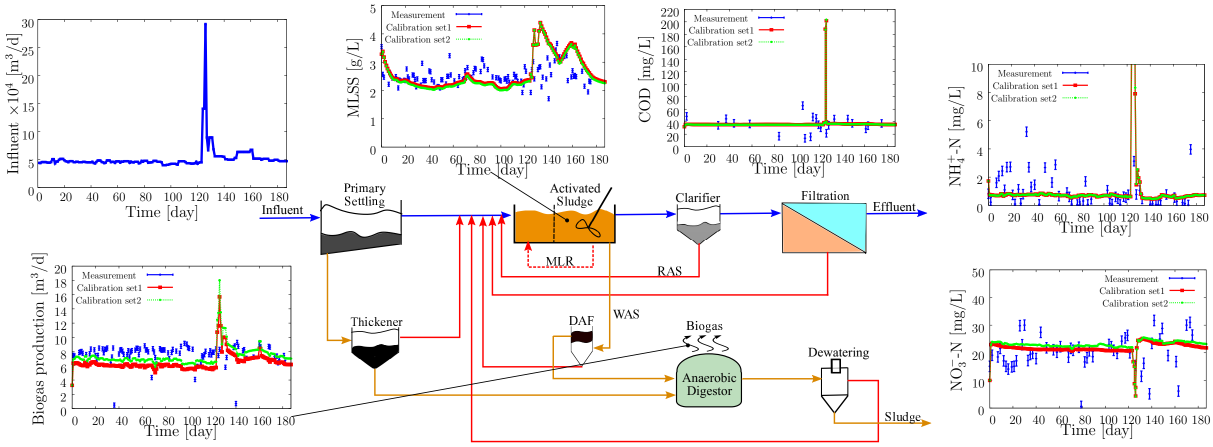



Figure 4.6: Calibration of effluent quality and biogas production in the WWTP. Calibration Set #1 (red trend line): mean COD and TSS influent from Table 2; Calibration Set #2 (green trend line): optimised influent COD and TSS.

4.5; the corresponding model predictions are shown in Figure 4.7 (red line). Here again, the main trend is well captured by the plant-wide model, although biogas production is underestimated by 25%. However, the predicted MLSS concentration in the aeration tank is well estimated during the same period, which possibly results from the same reason in that the mean COD and/or TSS influent concentration being underestimated. To confirm it, both influent COD and TSS concentrations have been estimated with their fractionation in a separate calibration. The results are presented in the Set #2 column in Table 4.5, with the corresponding model predictions shown in Figure 4.7 (green line). Similar trends are observed that the optimised influent COD and TSS concentrations are larger than the mean values within the standard deviation range, but this results in a large reduction in the biogas production rate mismatch.

Table 4.4: Summary of plant influent data for model validation.

| Details | Units | Median | StdDev [%] | Count |
|---|---|---|---|---|
| Alkalinity | mg $CaCO_3$/L | 231.0 | 14.6 | 6 |
| COD | mg/L | 494.0 | 47 | 6 |
| TSS | mg/L | 276 | 34 | 19 |
| $NH_4^+$-N | mg/L | 38.8 | 31 | 6 |
| Total nitrogen | mg/L | 51 | 28 | 6 |

Table 4.5: Calibrated parameters of wastewater influent and its fractionation with another 6 months data.

| Parameter | Unit | Set #1 | Set #2 |
|---|---|---|---|
| $f_{\mathrm{SI}}$ | g(COD)/g(COD) | 0.09 | 0.08 |
| $f_{\mathrm{SS}}$ | g(COD)/g(COD) | 0.16 | 0.10 |
| $f_{\mathrm{XI}}$ | g(COD)/g(COD) | 0.07 | 0.07 |
| $f_{\mathrm{XS}}$ | g(COD)/g(COD) | 0.68 | 0.75 |
| $f_{\mathrm{SND}}$ | g(N)/g(N) | 0.11 | 0.09 |
| $f_{\mathrm{XND}}$ | g(N)/g(N) | 0.09 | 0.11 |
| COD | mg/L | 494 | 600 |
| TSS | mg/L | 276 | 369 |

## 4.3 Plant-wide Analysis and Optimisation

The developed plant-wide model provides a means of quantifying effects of key operating variables on energy use/production and effluent quality in the WWTP. It can be also used to improve performance of the WWTP through systematic optimisation techniques based on mathematical programming. The following subsection gives more detail about the plant-wide optimisation problem formulation.

### 4.3.1 Optimisation Formulation

An informal statement of the optimisation problem for optimal operation of the WWTP is as follows: "Find the optimal operational decision variables minimizing the plant's

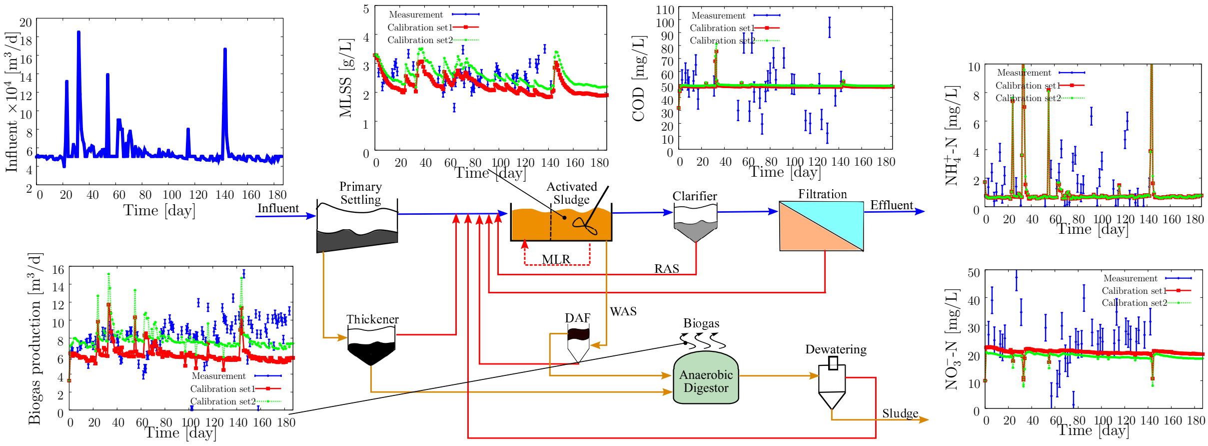



Figure 4.7: Recalibration of effluent quality and biogas production in the WWTP to verify the plant-wide model. Calibration Set #1 (red trend line): mean COD and TSS influent from Table 2; Calibration Set #2 (green trend line): optimised influent COD and TSS.

average energy consumption, while meeting the effluent regulations and satisfying the operational specifications."

The optimisation problem can be formulated as follows:

$$\begin{aligned} \min_{u} \quad & J(u) \\ s.t. \quad & \dot{z} = f(t, z(t), y(t), u(t)) \\ & g(t, z(t), y(t), u(t)) = 0 \\ & u^L \leq u(t) \leq u^U \\ & y^L \leq y(t) \leq y^U \\ & z^L \leq z(t) \leq z^U \end{aligned} \tag{4.4}$$

where $J$ is the objective function, $z(t)$ the vector of differential state variables, $u(t)$ the vector of control/manipulated variables, and $y(t)$ the vector of algebraic state variables, i.e. composite variables (e.g. COD, TSS, BOD, etc.). The differential and algebraic equations are equality constraints which can be described by a mass balance of the plant-wide wastewater treatment model. In this study, implementation of the plant-wide model is carried out in the general purposed modeling platform gPROMS, which has built-in optimisation capability to solve such optimisation problems. More detail for each component of the optimisation problem (4.4) is given below.

#### 4.3.1.1 Objective Function

The optimisation objective involves minimizing the net energy consumption, namely the difference between the average energy consumption of the main treatment/separation units and the average energy recovered from the biogas produced in the anaerobic digesters.

$$J = \bar{E}_{consumption} - \bar{E}_{production} \tag{4.5}$$

where $\bar{E}_{consumption}, \bar{E}_{production}$ are average energy consumption and energy recovered from biogas, respectively. energy consumption associated with both mixing and pumping is computed based on correlations derived from historical plant data. Due to the fact that data for calculation of pumping energy is not available, surrogate models through relationship between energy used and stream flowrate through pumps is developed. It is assumed that pumps were operated at constant efficiency for all flowrates; energy consumption for pumps can then be expressed as a function of flowrate through the pumps. Whereas, energy consumption of the aeration system and energy recovered from biogas produced are computed based on the relationships found in Gernaey et al. [164] as a first approximation:

$$AE = \frac{S_O^{sat}}{T \cdot 1.8 \cdot 1000} \int_{t=1}^{T} V \cdot K_L a(t) dt \tag{4.6}$$

$$ME = \frac{16 \cdot P_{atm}}{R \cdot T_{ad} \cdot T} \int_{t=1}^{T} \frac{Q_{gas}(t) \cdot p_{gas,CH_4}(t)}{P_{gas}(t)} dt \tag{4.7}$$

where $T$ is time duration, $AE$ and $ME$ are energy consumption from aeration and energy recovered from anaerobic digestion, respectively. $V$ is the volume of bioreactors; $P_{atm}$, $P_{gas}$, $p_{gas,CH_4}$ are atmospheric pressure, biogas pressure and partial pressure of $CH_4$, respectively ; $T_{ad}$ is the operating temperature of the anaerobic digester, and $R$ is the ideal gas constant. Note that energy consumption from aeration ($AE$) and energy production ($ME$) are part of the average energy consumption ($\bar{E}_{consumption}$) and energy production ($\bar{E}_{production}$) in Eq. 4.5.

#### 4.3.1.2 Effluent Standards and Operational Constraints

In order to cope with the current regulations of the Australian Environment Protection Authorithy (EPA), constraints are defined on BOD, TSS and $NH_4^+$-N concentrations in treated effluent, as given in Table 4.6. Note that satisfying these limits does not pose any particular problem with the current operation, at least during dry weather conditions (see Figure 4.6). Nonetheless, the quality standards are likely to be tightened in the coming years, especially with regards to nitrogen discharge (both $NH_4^+$-N and $NO_3^-$-N). Other constraints are defined on a range of control variables e.g. DO, WAS, RAS and MLR in order to account for equipment limits and/or in agreement with current engineering practice. Moreover, operational ranges are defined for two key process operation indicators, namely the sludge age (SRT) and the MLSS concentration. These limits and ranges are reported in Table 4.7 below.

Table 4.6: Effluent quality limits.

| Component | BOD mg/L | TSS mg/L | $NH_4^+$-N mg/L |
|---|---|---|---|
| max | 15 | 10 | 45.7 |

Table 4.7: Operational limits and ranges.

| Decision variables | DO mg/L | WAS $m^3$/day | RAS $m^3$/day | MLR $m^3$/day |
|---|---|---|---|---|
| min | 0.5 | – | – | – |
| max | 3.0 | 4,142.7 | 103,680 | 100,000 |
| **Operation variables** | **MLSS g/L** | **SRT day** | | |
| min | 2 | 7 | | |
| max | 5 | 15 | | |

#### 4.3.1.3 Decision Variables

Practical decision variables, e.g. variables that are commonly maniputed in WWTPs were selected to keep the optimisation results as practical as possible; Table 4.8 shows the selected variables and their nominal values. It should be noted that internal recycling of the mixed liquor from the aerated zone back to the anoxic zone is not currently used in this plant. In addition to the above variables, the effect of solids capture efficiency (SCE) in the primary sedimentation tanks were also considered. Although SCE is usually not manipulated in practice, one can easily imagine doing so by redirecting some of the primary sludge to the secondary treatment for instance (instead of the sludge treatment). Also, the addition of an external carbon source (methanol) for enhanced nutrient removal was also investigated.

Table 4.8: Decision variables and nominal values.

| Variable | Description | Nominal value | |
|---|---|---|---|
| DO | Dissolved oxygen setpoint | 2 | mg/L |
| WAS | Waste activated sludge | 2,272 | $m^3$/day |
| RAS | Recycle activated sludge | 58,000 | $m^3$/day |
| MLR | Internal recycle flowrate | 0 | $m^3$/day |

#### 4.3.1.4 Scenario-based Solution and Analysis

Instead of carrying out a single optimisation based on the foregoing problem statement, a scenario-based procedure is considered whereby variable discharge levels are imposed for $NH_4^+$-N or $NO_3^-$-N. Note that each scenario involves solving a separate (dynamic) optimisation problem, here using gPROMS. This procedure yields insight into the sensitivity of the optimal energy consumption, and corresponding operational decisions with respect to key discharge constraints, thereby providing a means for analyzing the interplay between energy consumption and effluent quality. In turn, this improved understanding helps determine improved strategies for energy saving and nutrient removal.

#### 4.3.1.5 Scenario-based Robust Optimisation

WWTPs are generally associated with uncertainty for various reasons such as natural variability, insufficient data and measurement errors [182]. A plant-wide WWTP model also consists of numerous uncertain parameters including influent conditions and kinetic coefficients for each unit process model. As a result, a number of problems have been arisen from model prediction accuracy to the risk associated with engineering decisions during design, upgrade or optimisation. While the results from nominal values are important to describe the qualitative features, it is important to account for uncertainty to improve the understanding of process phenomena, model prediction accuracy, and making solutions more practical. To deal with such problems, researchers have been working on various concepts of robustness which aims not to find the best solution to the nominal values (undisturbed systems), but to investigate a robust solution which is still good in the case of uncertain systems. In this study, the robustness is defined as the ability of the process to maintain its performance in an acceptable level although the actual parameters are different from the values assumed [182]. Once uncertainty has been considered explicitly during design and operation, it will provide more realistic results and enhance an understanding of specific phenomena. However, incorporation of uncertainty into wastewater engineering is less advanced compared to other fields, including a comprehensive discussion of sources of uncertainty, and evaluation methods applicable to wastewater treatment projects. Several attempts have been made to propose methods for the quantification of model prediction accuracy and uncertainty incorporated in model development and applications [183]. A scenario-based robust optimisation is a promising approach among alternatives such as Monte-Carlo simulation [184, 185]. This approach is computationally simple, easy to implement [186, 187], and can provide optimal operational conditions for a defined range of perturbations. For example, given that nominal wastewater influents in Table 4.1, or model parameters, may vary 10% in either direction, it would provide optimal conditions which an acceptable level of performance is maintained even though the nominal values are changed. This approach has been used in several studies and applications including the planning of a decentralized water supply and reuse system [187], robust model predictive control [188], and a water distribution system (WDS) [189]. Note that a scenario-based robust optimisation for the plant-wide WWTP model is still computationally difficult to incorporate all uncertain parameters because of a large number of variables, constraints and high nonlinearity. To reduce computational difficulties from the large scale optimisation problem (large nubmer of variables, constraints and high nonlinearity), only selected uncertain parameters and scenarios are incorporated.

### 4.3.2 Strategies for Reduction of Energy Consumption

In the current mode of operation, the plant-wide energy consumption is dominated by the aeration of the activated sludge reactors. Although partly compensated for by biogas production in the anaerobic digesters, this energy consumption appears to be relatively high compared to the current effluent quality, thereby suggesting good improvement potential.

The effect of varying the $NH_4^+$-N discharge concentration on the plant's minimal net energy consumption is presented in Figure 4.8a, and the corresponding optimal decision and operational variables are shown in Figure 4.8b. The optimisation results follow a similar trend for both calibration sets (see Section 4.2.3 and Table 4.3). Quantitatively, the larger organic load in Calibration Set #2 allows for a higher biogas production, and therefore a lower net energy consumption, compared to Calibration Set #1. Quite remarkably though, the optimal decision and operational variables are nearly identical, suggesting a certain robustness of the model-based predictions towards the uncertainty in influent composition. Especially clear from Figure 4.8a is the tight interplay between net energy consumption and $NH_4^+$-N discharge. For comparison, the actual plant's net energy consumption is estimated to be $2.18\times10^4$ kWh/day (daily average), and the treated effluent contains 0.9 mg($NH_4^+$-N)/L (daily average). Therefore, a reduction in the net energy consumption by around 20-25% could be achieved, through operational changes, without compromising the ammonia concentration in the effluent. Conversely, a reduction in the

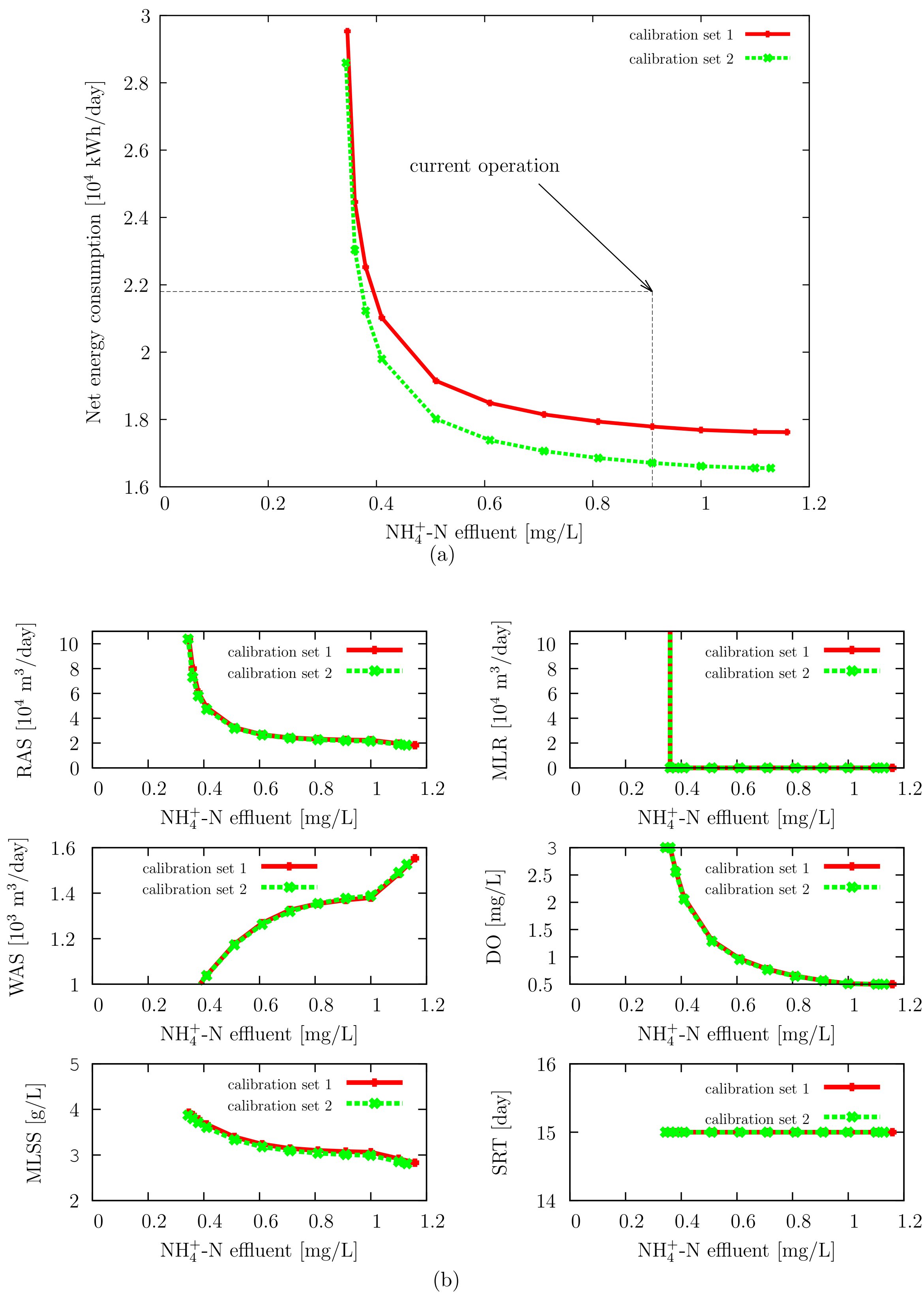



Figure 4.8: Effect of $NH_4^+$-N discharge level on (a) the net energy consumption and (b) on the decision/operational variables, for the two calibration sets in Table 4.3.

ammonia discharge by over 50% (0.4 mg/L) could also be obtained without increasing the net energy consumption. Overall, these results suggest that: (i) treating ammonia down to residual concentrations of approximately 1 mg/L may not increase energy consumption from the current level of energy consumption for this plant; (ii) a good compromise between energy saving and nutrient removal might be found for the plant as long as the ammonia discharge limit remains greater than approximately 0.6 mg/L, and; (iii) the plant may not produce an effluent with residual ammonia levels less than approximately 0.35 mg/L through operational changes only.

Closer inspection of the decision/operational variables trends in Figure 4.8b reveals that the optimal DO set-point increases significantly from 0.5 mg/L to 3 mg/L as the $NH_4^+$-N discharge concentration is lowered. Quite expectedly, the largest energy saving involves lowering the DO set-point to 0.5-1 mg/L here. Operating the activated sludge reactors at longer SRTs is also found to be advantageous from a plant-wide perspective, despite the corresponding reduction in biogas production due to a higher endogenous respiration and thus a lower sludge production (WAS flowrate). Conversely, the RAS flowrate increases significantly as the $NH_4^+$-N discharge concentration is reduced, thus maintaining an optimal MLSS concentration around 3 g/L. Finally, the optimal strategy does not involve recycling the mixed-liquor back to the anoxic zone since high limit is currently defined with regards to TN discharge, and an increased MLR would entail extra pumping costs.

It can be clearly seen that the net energy consumption is dominated by aeration energy, and hence a lower DO set-point can significantly reduce the net energy consumption while effluent quality is still satisfied. However, it is not widely accepted in practice to reduce the DO set-point below 2 mg/L to handle uncertain situations such as large fluctuation of the flowrate, and/or influent concentrations. The effect of varying $NH_4^+$-N discharge concentration at the constant DO set-point of 2 mg/L on the net energy consumption was also investigated. The result is presented in Figure 4.9a, and the corresponding optimal decision and operational variables are shown in Figure 4.9b. A reduction in the net energy consumption of around 13% could be achieved, through operational changes, without changing the DO setpoint (2 mg/L) and enhancing $NH_4^+$-N removal performance in the effluent over 50% (0.44 mg/L). It is also found that the decision/operational variables follow the same trends as in Figure 4.9b when the $NH_4^+$-N discharge concentration is varied.

Another interesting study was to investigate the feasibility of incorporating uncertainty into a plant-wide model to robustify plant-wide model predictions through the application of a scenario-based robust optimisation that directly accounts for the uncertainty. Here, COD and TSS in the wastewater influent are selected as uncertain parameters because it was found in Section 4.2.3 that COD and TSS have high standard deviations from measurements, and both parameters are likely to be the main cause of the observed mismatch between the predictions and measurements. Initially, two uncertain parameters (COD represented by $\theta_1$ and TSS represented by $\theta_2$) were perturbed within 0-15% from the nominal values (Table 4.1), and then 5 scenarios were generated for each perturbation shown in Figure 4.10a to explore the optimal condition at a given range of perturbations to enhance robustness. However, to prove that these 5 scenarios are a set of representative ranges of plausible uncertain parameter values, the other 5 sampling scenarios were also included, as illustrated in Figure 4.10b (5 more points in the box). Then, the 5 scenarios (the nominal and perturbed values) are optimised simultaneously compared to the 10 scenarios (the nominal, perturbed values and sampling points). Figure 4.11 shows a comparison between two cases (5 and 10 scenarios). Both cases follow a similar trend for the net energy consumption, and the optimal decision/operational variables are also found to be identical. Therefore, the first case (5 scenarios) is used subsequently in order to robustify the optimal operational strategies in the presence of uncertainty.

Figure 4.12a shows the plant's minimal net energy consumption at various $NH_4^+$-N discharge levels when the uncertain parameters 0-15% perturbations are taken into account; the corresponding optimal decision and operational variables are reported in Figure 4.12b.

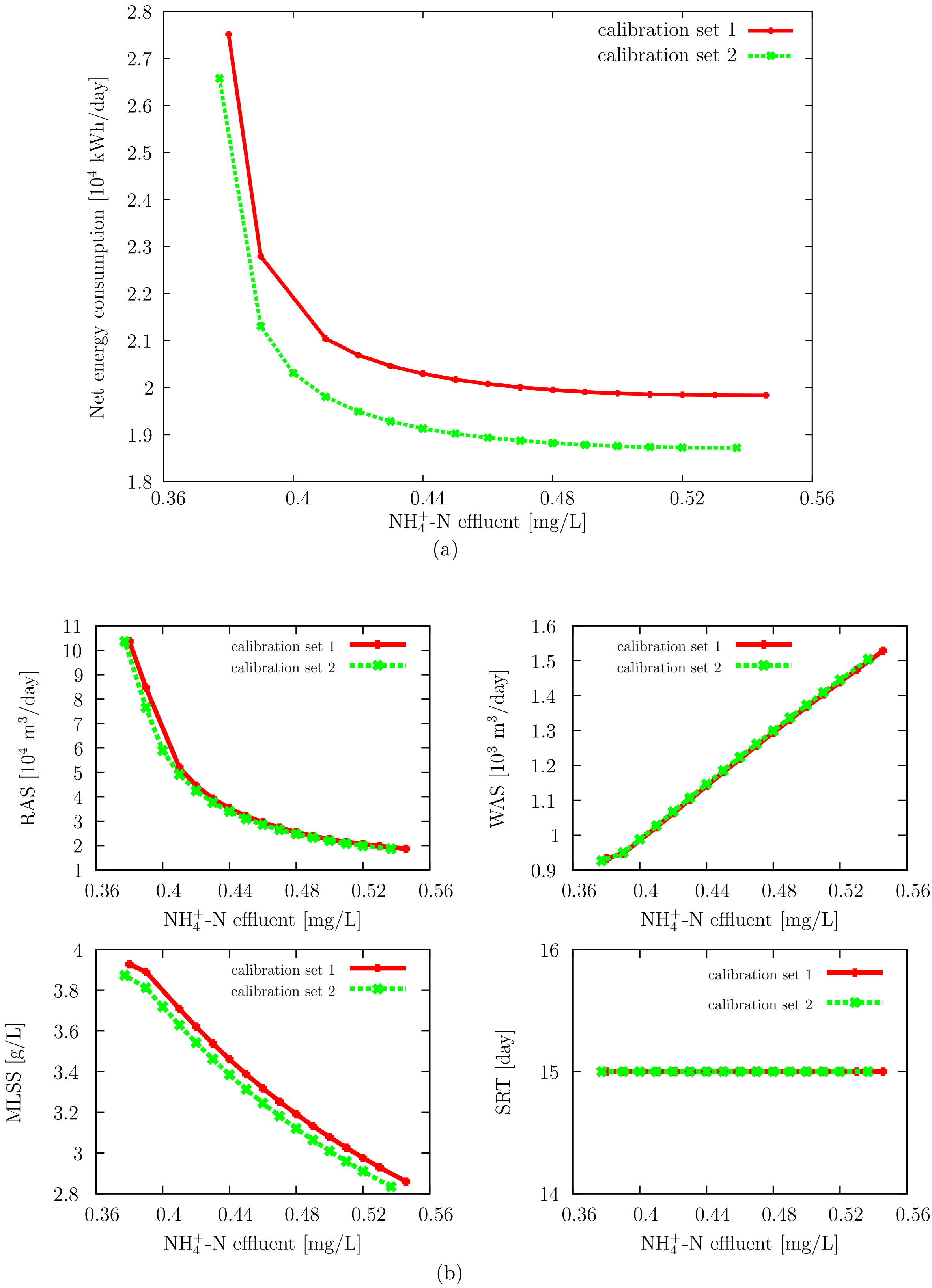



Figure 4.9: Effect of $NH_4^+$-N discharge level on the net energy consumption when the DO setpoint is fixed at 2 mg/L (a) and the decision/operational variables (b), for the two calibration set in Table 4.3.

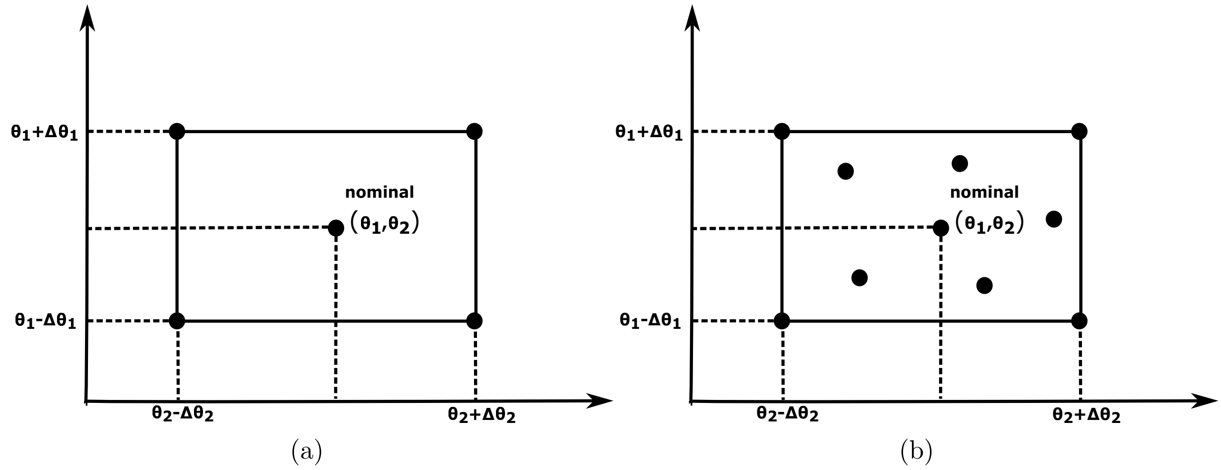
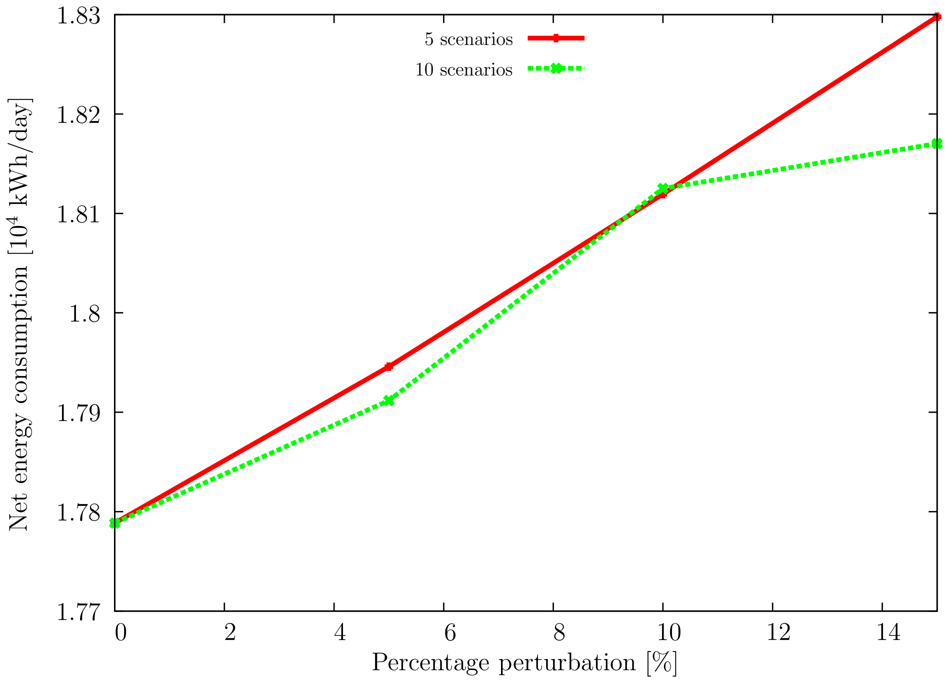
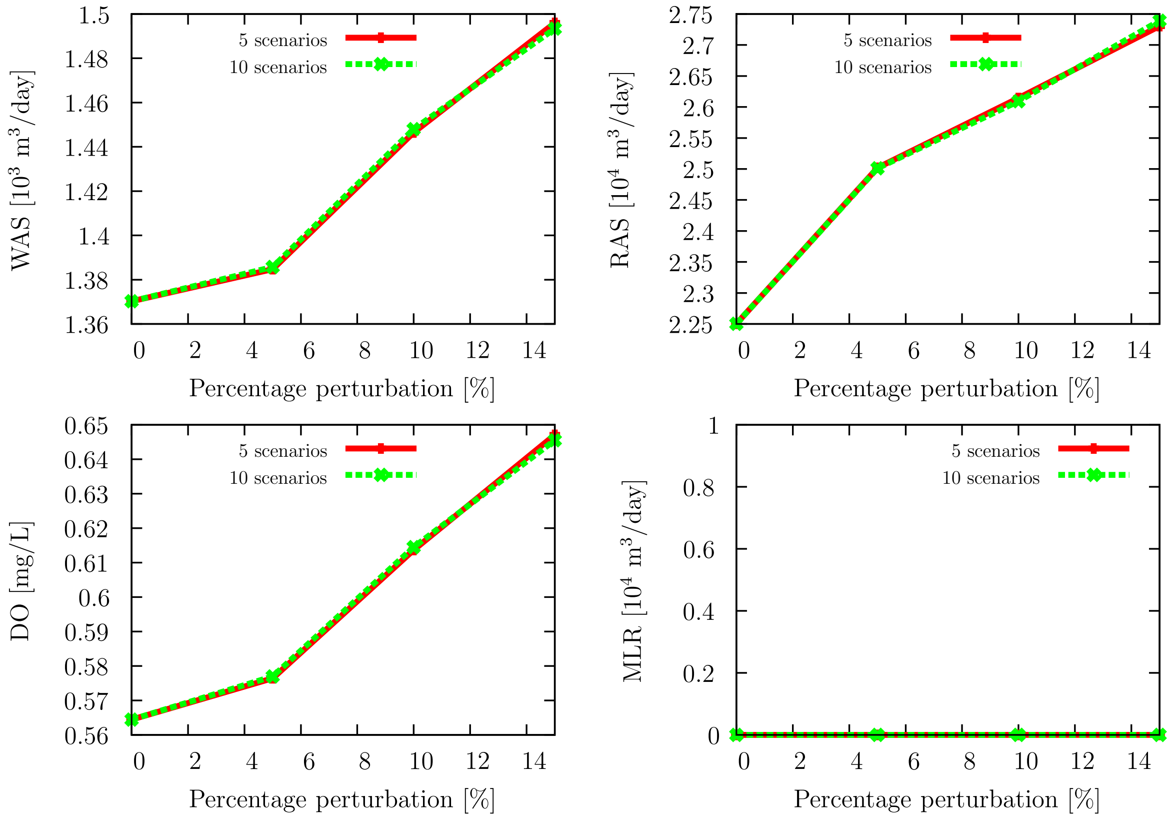



Figure 4.10: Scenario generation after perturbation (a) the perturbed values and the nominal value (b) the perturbed values, the nominal value and the sampling points (5 points in the box). $\theta$ in this study is referred to uncertain parameters (COD and TSS)

The results show a similar trend for a given range of perturbations, but different magnitudes; the larger the plant is perturbed by uncertain parameters (COD and TSS), the higher the net energy consumption. Apparently, there is a trade-off between the plantwide's minimal net energy consumption and robustness. This is because the scenario-based optimisation needs to provide larger flexibility within the system to allow it to adapt to a range of uncertain events at reasonable net energy consumption. The optimal conditions need to provide the best operational strategies to best fit all scenario constraints (effluent quality and operational constraints) as closely as possible while still maintaining feasibility. Closer investigation of the decision/operational variable trends in Figure 4.12b shows that they follow similar trends to the previous study when the $NH_4^+$-N discharge level is varied. But whereas the WAS and MLR flowrates and the DO set-point are rather insensitive to the level of uncertainty, the RAS flowrate increases more appreciably in the robust solution, thus providing a means of counteracting uncertainty in the influent concentration.

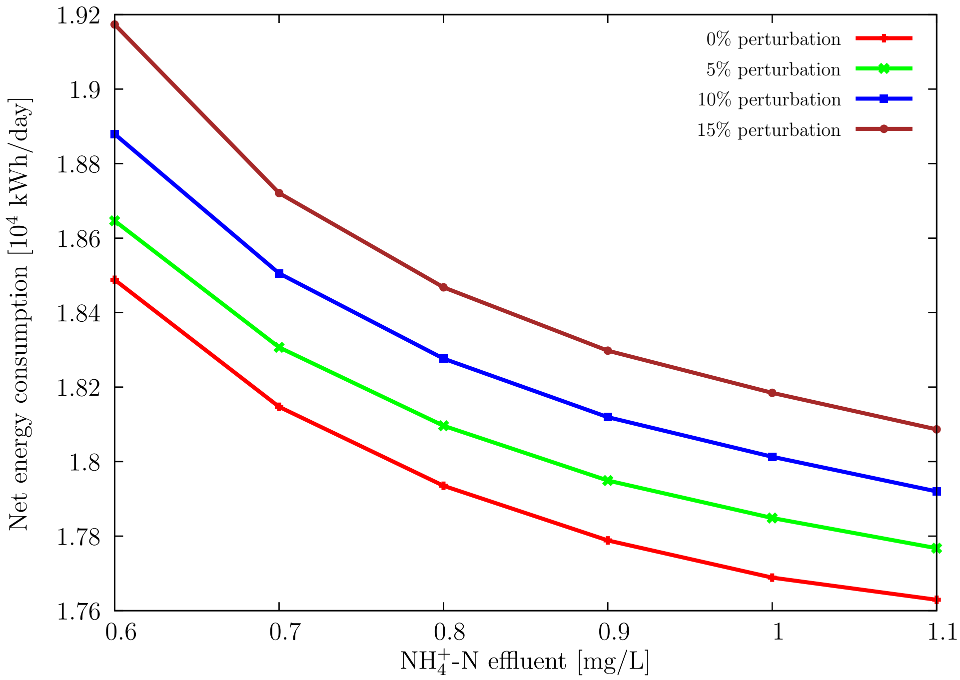



(a)

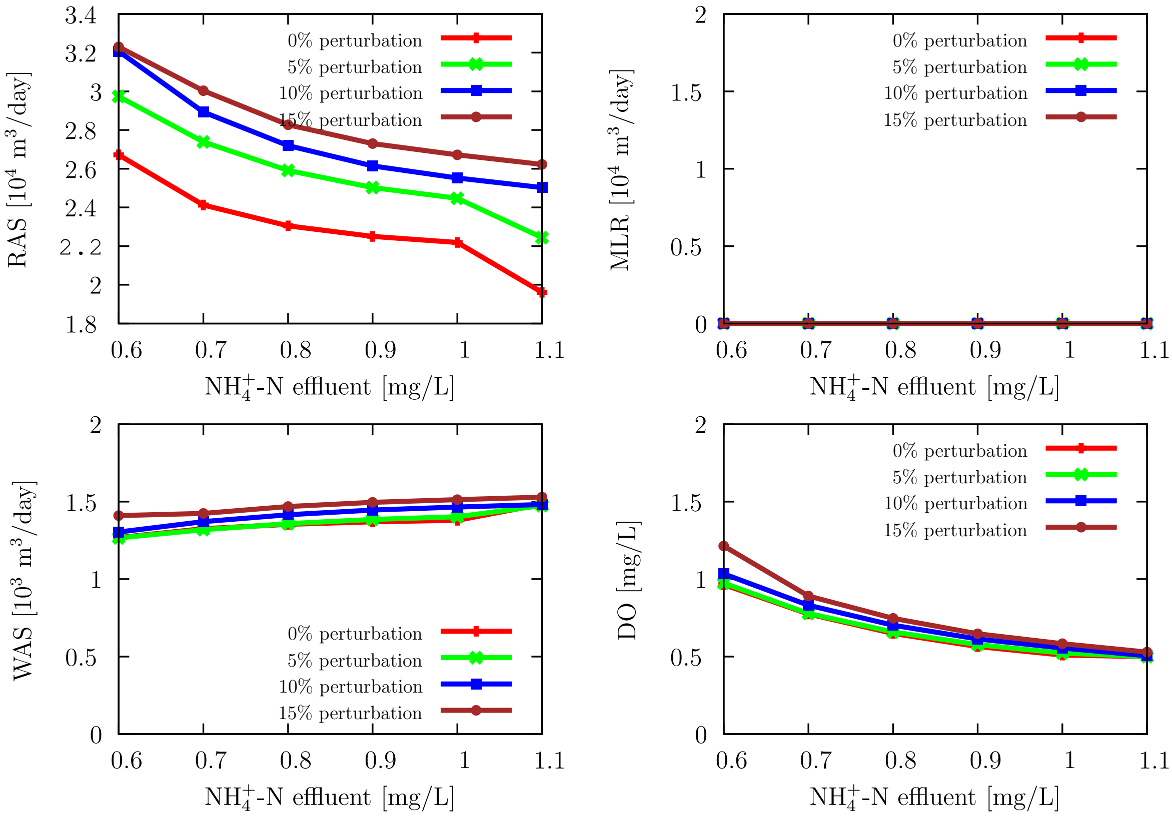



(b)

Figure 4.11: Comparison of the scenario-based robust optimisation for 5 scenarios and 10 scenarios (a) the net energy consumption, (b) the decision/operational variables.




(a)

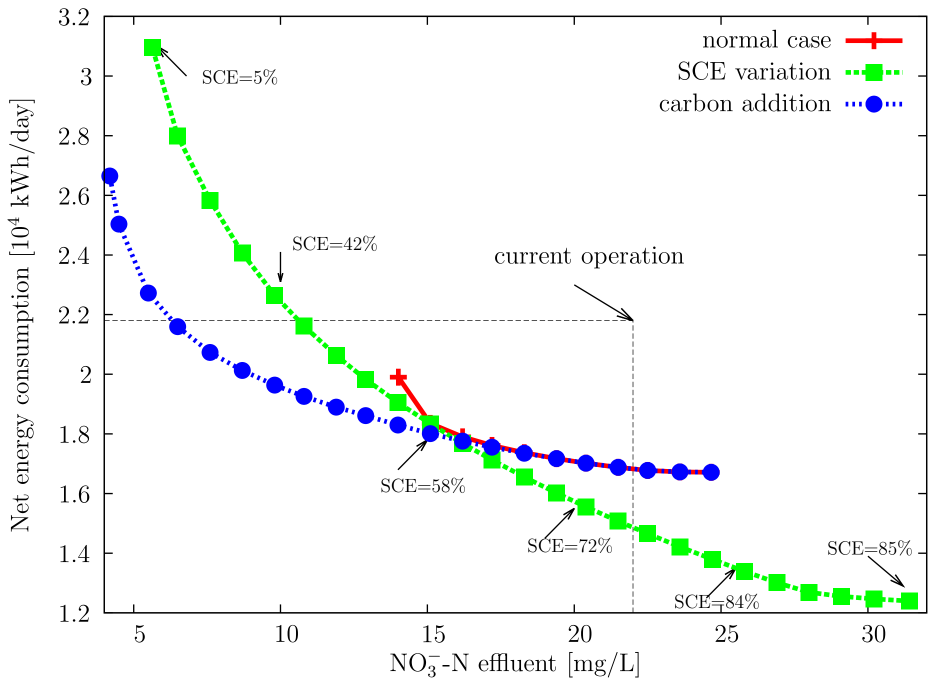



(b)

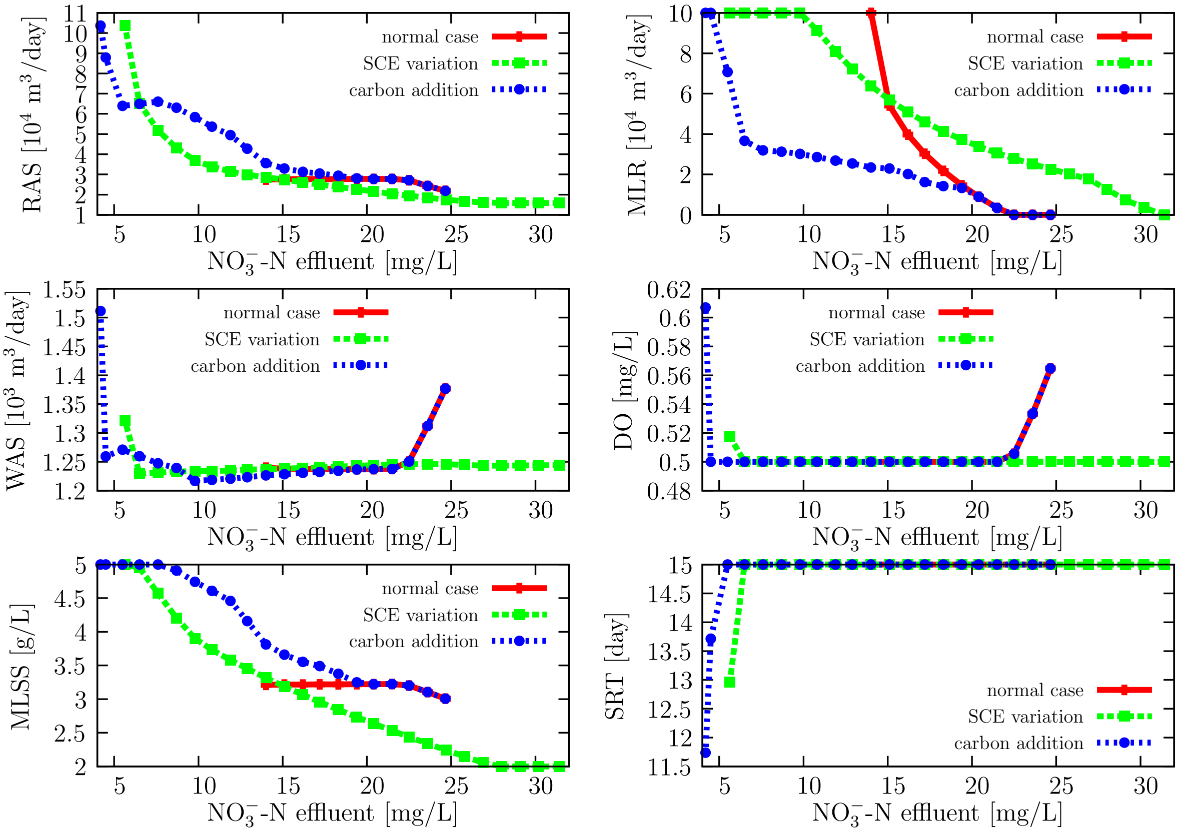
Figure 4.12: Effect of ammonia discharge level on the net energy consumption (a) and on the decision/operational variables (b) under the presence of uncertainty.

### 4.3.3 Strategies for Enhanced Nutrient Removal

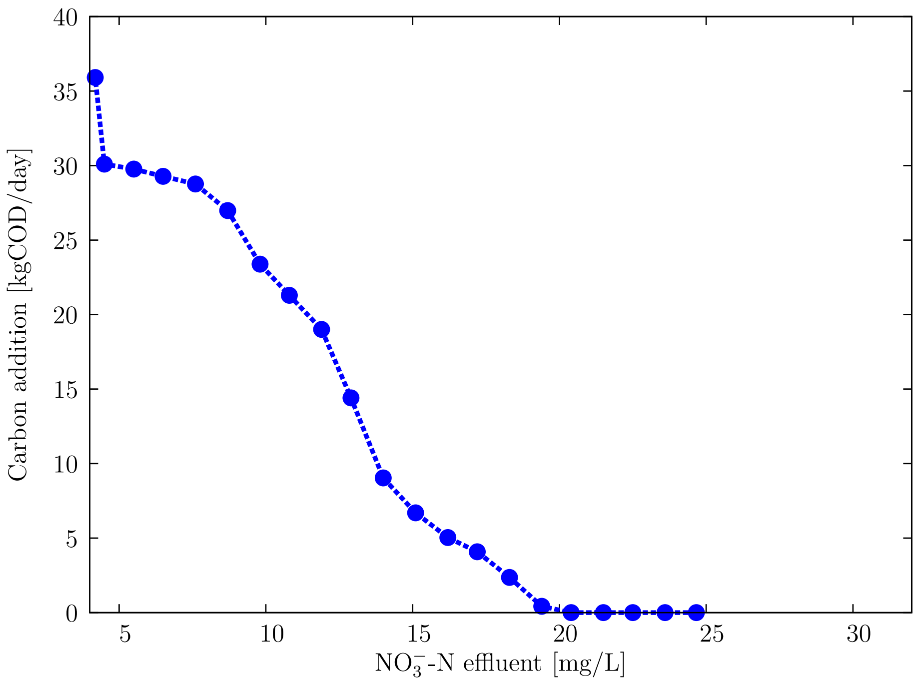
Because residual $NH_4^+$-N levels are already quite low, typically less than 1 mg/L, most of the potential for enhancing nutrient removal lies with reducing $NO_3^-$-N levels. This section investigates to what extent such reductions can be achieved through operational improvements. The effect of varying the $NO_3^-$-N discharge concentration on the plant's minimal net energy consumption, at a constant $NH_4^+$-N discharge concentration of 0.9 mg/L, is presented in Figure 4.12a; the corresponding optimal decision and operational variables are reported in Figure 4.12b. Note that these results are based on Calibration Set #2 (see Section 4.2.3), and turn out to be similar to those produced with Calibration Set #1. Moreover, the three curves on the plots correspond to the optimal operation in terms of the decision variables DO, RAS, WAS and MLR, without (red solid line), with (green dotted line) SCE as an extra decision variable. The nominal value of 55% capture efficiency was used in the former case and addition of external carbon source (blue dotted line).



(a)




(b)




(c)

Figure 4.12: Effect of nitrate discharge level on the net energy consumption (a), on the decision/operational variables (b) and on the amount of carbon addition (c), at constant ammonia discharge level of 0.9 mg/L and for Calibration Set #2 in Table 4.6.

As previously with $NH_4^+$-N discharge, Figure 4.12a shows a tight interplay between net energy consumption and $NO_3^-$-N removal. For comparison, the current plant's net energy consumption is estimated to be $2.18 \times 10^4$ kWh/day (daily average), and the treated effluent contains as much as 22.1 mg/L (daily average). The optimisation results suggest that a reduction of the $NO_3^-$-N concentration down to approximately 14 mg/L could be obtained without increasing the net energy consumption, through operational changes. These changes involve increasing the recirculation of mixed-liquor back to the anoxic zone as a source of carbon for denitrification; mainly an increase in the MLR flowrate here. In this instance, the additional pumping energy is balanced by a reduction of the compression energy (DO set-point down to 0.5 mg/L).

Regarding solid capture efficiency, a lower SCE means that a larger fraction of particulate organic pollution entering the plant will be sent to the secondary treatment, thereby increasing the amount of carbon available for denitrification in the anoxic tanks. On the other hand, the BOD load sent to the anaerobic digester will decrease, which in turn will decrease biogas production. These considerations explain why $NO_3^-$-N concentrations lower than 10 mg/L could be achieved if the SCE were to be reduced to <42%, with a slight increase in the net energy consumption of the plant (around 5%). In practice, this strategy should be compared to the direct addition of a fresh carbon source (e.g., methanol) in the anoxic tanks.

Addition of external carbon source (methanol) was also studied to investigate its effect on nutrient removal. The results show that greater nutrient removal could be achieved through the addition of external carbon, and an increased flowrate of recycling streams (MLR and RAS) to send back $NO_3^-$-N to the anoxic zone for denifrification. A reduction in $NO_3^-$-N concentration can be lower than 5 mg/L, thereby increasing amounts of carbon addition (see Figure 4.12c), although this would be at the cost of around an 18% increase in the net energy consumption of the plant because of no limitations in organic matter available for denitrification. However, it turns out that the net energy consumption is lower compared to variation of SCE because addition of external carbon does not need to compromise the amount of sludge sent to anaerobic digestion, unlike a variation in SCE. Note that using an external carbon source can incur addtional costs with regard to chemicals, which is not considered in this case.

## 4.4 Summary

This chapter has presented the application of a systematic model-based optimisation to a full-scale activated sludge plant combined with anaerobic sludge digestion. The objective was to quantify the effect of key operational variables on effluent quality and energy consumption, and to determine improved operational strategies to take account of these conflicting objectives. Overall, the model-based optimisation can be used to simultaneously adjust the key operating variables to optimise the WWTP's performance compared to the current studies, i.e. adjusting one operating variables at the time and the optimal solution is not guaranteed. Similar to the previous study, it is used to inform what point of nutrient discharges uss significant amount of energy to identify the main trade-off between two conflicting objectives. It is also possible for model predictions to incorporate the uncertainy into the optimisation framework to robustify the operational strategies. Although the results observed are only specific for this case study, the concept of systematic optimisation based on plant-wide models together with a scenario-based robust optimisation can be applied to other wastewater treatment systems to develop the optimal operational strategies with enhanced robustness. The results of the scenario-based optimisation show good potential for further improvements, with reduction in energy consumption of around 20-25% through operational changes (DO set-point, and WAS, RAS and MLR flowrates) if the effluent targets were to remain at the same level. It was also found that the $NO_3^-$-N concentration in the effluent could be reduced to less than 15 mg/L with no increase in net energy consumption. Our analysis suggests that the $NO_3^-$-N concentration could even be reduced to 10 mg/L or less by decreasing the solids capture in the primary sedimentation tanks to only 42%, subject to a small increase in net energy consumption. Finally, addition of an external carbon source (methanol) can provide better performance in terms of greater $NO_3^-$-N removal, and lower net energy consumption compared to the case of solids capture variation. A reduction in $NO_3^-$-N concentration to lower than 5 mg/L subject to an 18% increase in net energy consumption.

# Chapter 5

# Synthesis of Wastewater Treatment and Recovery Facilities using Superstructure Optimisation

## 5.1 Introduction

Wastewater has been considered a human health concern and environmental hazard for a long time. Most wastewater treatment designs are based on engineering traditions established back in the early $20^{th}$ century [15]. To produce an effluent that was of satisfactory quality for discharge into the environment, processes were developed which used large amounts of energy and land, and produced large amounts of sludge; however, a paradigm shift is underway towards making wastewater treatment facilities more sustainable. In this new paradigm, wastewater is regarded as a renewable resource from which water, materials and energy can be recovered, thereby forcing "wastewater treatment" to transit towards "resource recovery" facilities [16]. It has even been argued that the design of wastewater facilities could have a significant impact on reducing greenhouse gas emissions [190]. Until recently a majority of the activities related to resource recovery from wastewater have focused on waste sludge streams, which are a by-product of biological treatment.

Because these streams have relatively low flows in comparison to the main wastewater stream, and are more concentrated, resources can be recovered from them with minimal changes to the wastewater treatment infrastructure. For instance, mesophilic anaerobic digestion of primary and waste-activated sludge produces a methane-rich gas which is being used in most treatment facilities worldwide to recover energy. It has been reported that a quarter to half of the energy requirements for an activated sludge facility can be provided by such energy recovery systems [66, 191].

It is now recognized that wastewater is a potential source of valuable resources, and technologies required for resource recovery are maturing. Apart from the barrier of technological and market penetration, a lack of design methodologies and decision-making tools are also a significant problem in being able to evaluate the most sustainable facility in a given geographic and cultural context. Several studies have investigated the possibility of designing a new wastewater treatment facility to select the optimal process configuration. Sutton et al. [103] developed a new municipal wastewater treatment flowsheet with the aim of achieving sustainability though energy, water and nutrient recovery, as shown in Figure 5.1. The new flowsheet consists of an aerobic membrane bioreactor

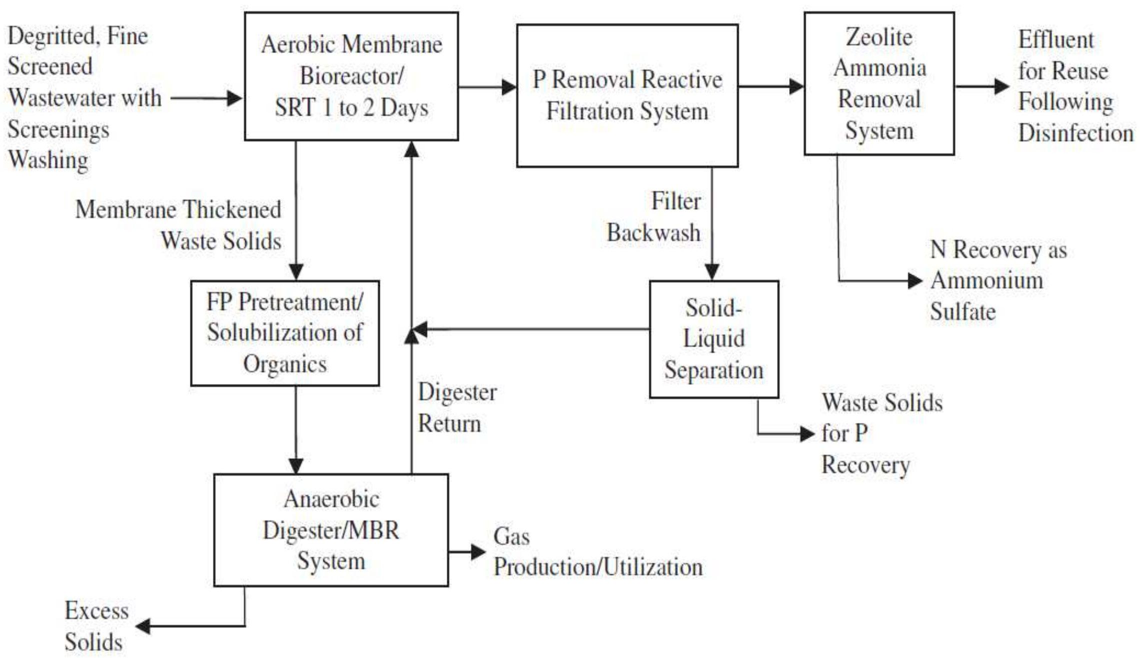



Figure 5.1: Schematic representation of the new flowsheet [103].

coupled with an anaerobic MBR digestion system where energy can be recovered, and physical-chemical systems (reactive filtration and zeolite ammonia removal system) to recover nutrients. It is found that the modeling results support the new flowsheet in terms of economic and environmental advantages compared to the conventional approach. However, a number of questions arose regarding the selection of treatment/separation units and their interconnections from a wide variety of unit operations that are available. This question is known as flowsheeting or synthesis in process engineering. It should be mentioned that there are also other factors used to design wastewater treatment treatment facilities which are not considered, e.g. skill of operators, funding availability for the simplicity reasons. More detail or factors can be added in the future study to make it more practical.

In order for the synthesis of sustainable WWTPs to be feasible, it is necessary to account for the trade-offs between capital, operating costs and sales, while water quality, and other environmental considerations also need to be satisfied. Although technical considerations can significantly decrease the combinatorial problem and enable us to select the promising solutions, they typically do not provide all the information required for an optimal system. As the array of technical options grows, a simple enumeration of all possible alternatives quickly becomes unmanageable, quite apart from the fact that each technology has its own parameters to specify or optimise. In this chapter, we advocate the use of systems engineering methods and tools to address this problem in a systematic way. A superstructure modeling approach [19] is considered which can account for a large number of treatment and separation options (units), along with all the feasible interconnections between them. Rigorous optimisation based on such a superstructure leads to mixed-integer nonlinear programs (MINLPs) that can be implemented and solved using state-of-the-art mathematical optimisation software such as GAMS (`http://www.gams.com`). However, the key to the success of this methodology is the development/selection of mathematical models for the units that are simple enough for the optimisation problem to remain tractable, yet provide reliable estimates of their performance and associated costs. The remainder of this chapter is organised as follows: Section 5.2 describes the superstructure approach, and focuses on the performance models for the treatment/separation units, and assessment criteria. Section 5.3 presents the optimisation formulation including material balances and optimisation techniques used to solve the superstructure-based optimisation. The proposed methodology is illustrated by the synthesis of a simple resource recovery facility in Section 5.4.

## 5.2 Methodology

In chemical processes where advance technologies for process design and operation are well developed, design methodology can be divided into two main approaches: traditional-conceptual [192, 193], and superstructure optimisation-based approaches [19]. The former relies on the existence of a natural hierarchy among engineering decisions, which are made during the generation of a process flowsheet. This approach is widely used because the complexity of process synthesis is relatively low where subprocesses of a plant are designed sequentially without considering interactions between the different stages. Specific conceptual tools are also developed to support the design of particular subprocesses through graphical representations based on thermodynamics, such as the use of residue curves to design of distillation-based separation, and the use of pinch technology to design heat exchanger networks. In the superstructure optimisation-based approach, a network consisting of all potentially feasible unit operations and relevant interconnections, known as a superstructure, is initially taken into account. Then, this superstructure is used to formulate an optimisation model including reformulated unit models, interconnections and relevant constraints. Such a model generally includes binary selection to allow us to select/deselect the unit operations and their interconnections. This approach has been applied to several scenarios, especially water network synthesis to minimize fresh water consumption, and wastewater generation through regeneration and recycle/reuse [194, 21, 22].

More specifically, the synthesis of wastewater treatment facilities is the selection of treatment/ separation processes which treat wastewater to satisfy the standard regulations before being discharged into the receiving waters. There are several factors considered in designing wastewater treatment processes [17], and the number of treatment/separation unit alternatives have been increasing steadily. The design of wastewater treatment processes relies mostly on knowledge-based systems [145], and heuristic rules based on experience [17], that are used for the selection and ordering of wastewater treatment units; however, they cannot guarantee an "optimum" solution. The systematic superstructure optimisation-based approach can be ideally effective because a large number of process alternatives are considered, and it can optimise the optimal process configuration and its operational conditions.

### 5.2.1 Superstructure-based Optimisation

Superstructure modeling and optimisation is at the core of the synthesis of sustainable wastewater treatment facilities. In this work, surrogate models have been applied to generate simple, yet reliable models to reduce the inherent complexity of wastewater treatment models. The proposed methodology is illustrated in Figure 5.2. The most promising alternatives would in turn be validated against the performance and cost predicted by the wastewater treatment simulator. Typically, this would create an iteration between the superstructure optimisation and the simulator in order to refine the regression models as appropriate. In particular, recent developments in surrogate-based optimisation can guarantee an overall optimum with minimum recourse to detailed models [195, 196]. Finally, the selected process candidates would be considered for detailed performance and cost analysis, including integration options and operability issues. Here again, further iterations with the superstructure optimisation block could prove necessary in order to account for additional design and operational constraints. The focus in this chapter is more specifically on the components in the gray-shaded area of Figure. 5.2. The main objective of the following case study is to provide a proof-of-concept of this superstructure optimisation approach based on simple regression models, while also showing that the underlying optimisation problems are indeed tractable to produce guaranteed global optimality. An extension of this approach to incorporate LCA considerations, along with a more complex case study in municipal wastewater treatment, will be presented later on in Chapter 6.

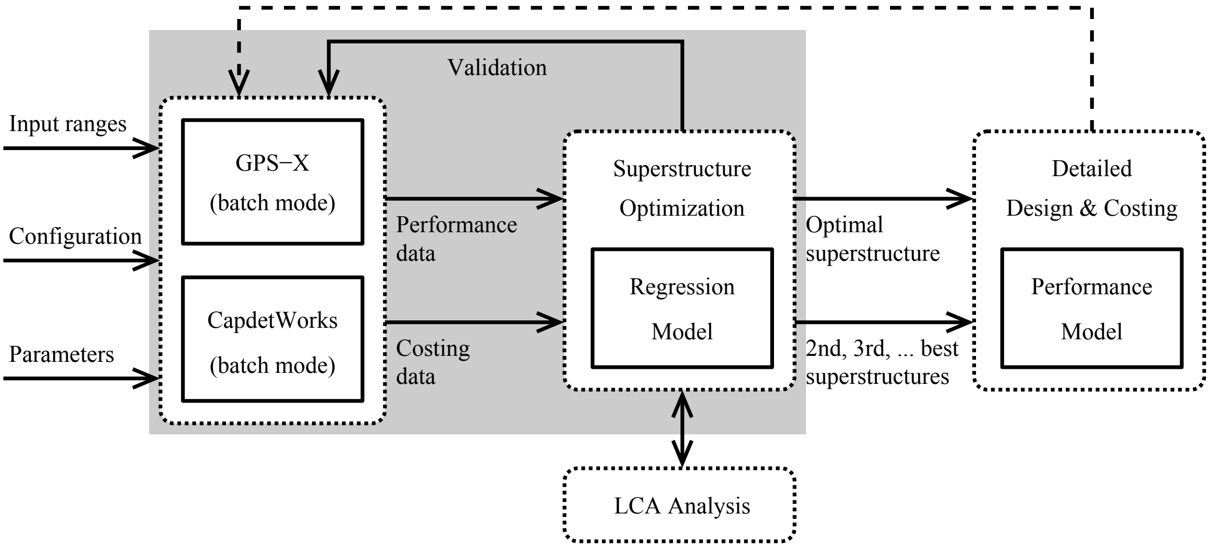



Figure 5.2: Illustration of the proposed methodology based on superstructure optimisation and regression models.

## 5.2.2 Surrogate Model

To address challenges associated with complexity in wastewater treatment facilities, and their interactions, the whole process/plant needs to be disaggregated into smaller process groups. This approach allows us to handle highly complex models and reduce the complexity of optimisation problems. The model generated from the smaller or less complex systems can then be used to formulate the superstructure-based optimisation problem to determine process alternatives and their interconnections. After disaggregating the complex proceess into the smaller process groups, it is the role of the mathematical models of each treatment/separation unit to predict their performance. In compliance with the superstructure optimisation method and current capabilities of optimisation technology, these models must remain as simple as possible, typically linear, piecewise-linear or polynomial relationships between the input/output variables. Currently, the direct use of complex biodegradation models such as ASM1-3 [110] and ADM1 [114] for the bioreactor, or complex crystallization, adsorption and filtration model for the separation units for performance prediction in the superstructure is intractable from a computational standpoint. The simple and widely used approach is to assume fixed conversion, removal or split fractions in the treatment/separation units, and such an approach is typically used in water network synthesis (see, e.g. Khor et al. [22]). In this work, an alternative, potentially more accurate method relying on detailed first principle models, as performed in wastewater treatment simulators such as GPS-X®, is developed. This is known as the surrogate model or the response surface model. The surrogate model is defined a simplified approximate model mimicing the behavior of the high fidelity model. Based on data generated by a simulator, either at steady state or averaged over a cyclic steady state, for various influent compositions (COD, TSS, etc.) and given operational parameters (HRT, SRT, etc.), simple regression models can be fitted to the simulated data. It should be noted that the validity of generated surrogate models is limited to certain ranges based on simulation ranges, and the bounds of such ranges should be included in the problem formulation to ensure that the surrogate models are valid. However, this approach may fail to obtain the optimal solution, or the solutions are very different from the integrated system; to overcome such problems the surrogate model, including simulated ranges, needs to be updated every time the solution is found. Different techniques are used to develop a surrogate model based on the complexity of the treatment/separation units. For the units with less complexity, the simplified model can be used as a surrogate model directly.

As the first principle models of wastewater treatment processes are highly complex, the surrogate models generated need to be accurate enough while maintaining simplicity to make the superstructure-based optimisation problem tractable. Such surrogate models can be derived using data obtained from simulated or experimental data of individual units/models. In this work, the commercial wastewater process simulator, GPS-X®, was used to generate the necessary data from the treatment/separation units to predict the behaviour of the disaggregated units. Having the simulated or experimental data, it is important to generate the surrogate or the simplified approximate model. Polynomial regression including linear, piecewise, and quadratic is the simplest technique and widely used in several applications [197]. The approximation of polynomial regression can be generally written as [198]:

$$y(x^{(i)}) = \sum_{j=1}^{K} a_j \nu_j (x^{(i)}) \tag{5.1}$$

Or it can be presented in the matrix expression

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{A} \tag{5.2}$$

where $\boldsymbol{y} = [y(x^{(1)} y(x^{(2)} ... y(x^{(p)}]^T$ is a vector of observed responses (simulated or exmperimental data), $\boldsymbol{X}$ is a matrix of the basis functions, $p$ is the number of simulated or experimental data or sampling point. $\boldsymbol{A}$ is a vector of estimated polynomial regression coefficient which can be calculated as follow:

$$\boldsymbol{A} = (\boldsymbol{X^T X})^{\boldsymbol{-1}} \boldsymbol{X^T y} \tag{5.3}$$

The first-order polynomial model (linear) is the simplest example of polynomial regression.

$$y(x) = y([x_1, x_2, ..., x_n]^T) = a_0 + \sum_{j=1}^{n} a_j x_j \tag{5.4}$$

where $y(x) = y([x_1, x_2, ..., x_n]^T)$ is the observed responses and $a_0, a_j$ are the linear regression coefficient. Figure 5.3 shows an example of the methane conversion efficiency in a UASB reactor as predicted by the ManTIS2 model in GPS-X® for various HRTs, along with a corresponding piecewise-linear regression model using in the superstructure model.

Some disaggregated models which are simple enough can be used directly in the optimisation framework. For example, an ideal separation model is used to reduce the amount of the particulate fraction in the wastewater stream, and to concentrate the particulate fraction in the sludge stream. The model is already simple because of several assumptions, e.g. no reactions occurring in the system, and is typically controlled by two parameters:

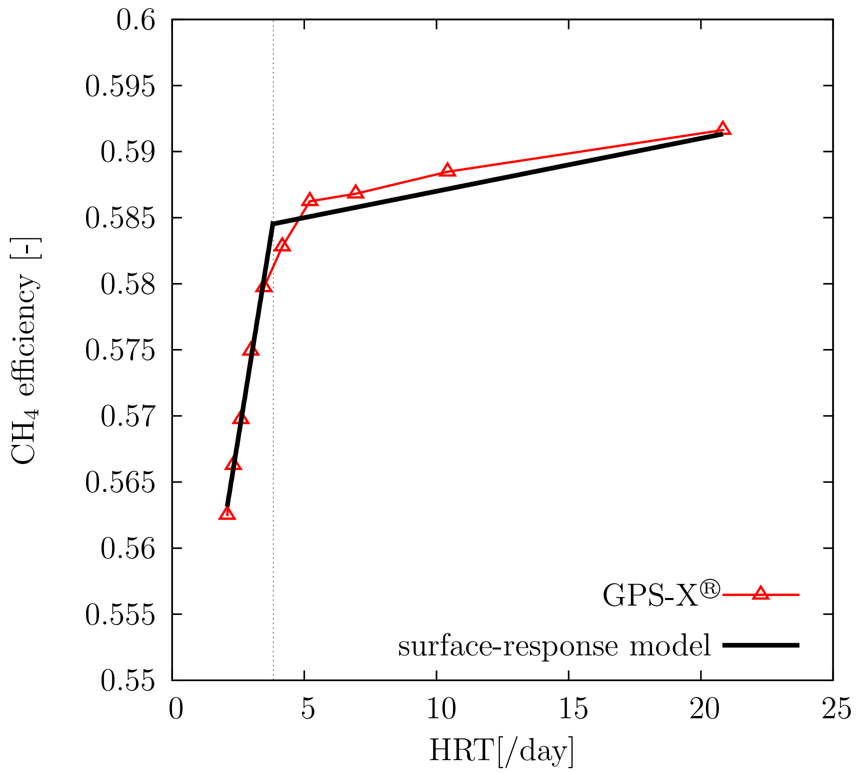



Figure 5.3: Illustration of a piecewise-linear performance model obtained from GPS-X® simulated data.

the split fraction and TSS removal efficiency. The soluble fraction is not affected, and equal to the inlet stream for the outlets of water and sludge streams; it appears that this model is simple enough and can be used in the optimisation problem directly.

Similar to the performance of disaggregated treatment units, reliable costing information (both CAPEX and OPEX) can be obtained from preliminary costing software such as CapdetWorks®, or data from the literature or provided by practitioners. Data can be generated by such programs for various units and/ or flowrates and make a surrogate model to obtain a simple linear, piecewise-linear or polynomial models. Note that the actual cost for CAPEX and OPEX which can be from different companies/people is suggested to be used for analysis to make the results more practical. However, the actual data is sometimes not available. Instead, the approximated cost is used and it is worth pointing out that using a common source and methodology for costing various technologies is advantageous in terms of consistency. In this study, CapdetWorks® can provide cost information including construction, energy, material, labor and chemical costs. The cost estimates are based on national indices (not site specific) and equipment cost databases in U.S. Different countries may have different cost databases and this can lead to different solutions. For example, land cost in some countries may be significantly high compared to other costs, e.g. equipment and energy cost so the optimal solution obtained is likely to use a small area of land but may use high energy. Some countries, however, may have a high energy cost compared to land cost are likely to obtain the optimal solution that uses lower amount of energy.

### 5.2.3 Problem Statement

The synthesis problem statement starts with the specification of the following data:

- A set of wastewater influents of given flowrates and composition,
- A set of water sinks with known maximum concentration limits e.g. local regulations,
- A set of treatment/separation units with given performance for target compounds.

These specifications can be represented by a generic superstructure in which every possible interconnection in a fixed network topology is considered. The superstructure is illustrated in Figure 5.4 for a simple network topology that consists of a single wastewater stream, a single water sink and a set of treatment/separation units. The objective of the synthesis problem is to determine an optimal resource recovery facility in terms of; (i) its units, (ii) the piping interconnections between the units, and, (iii) the flowrates and compositions in the interconnections. The mathematical model of integrated process wastewater treatment facilities consists of mass balance equations for selected components for every treatment/separation unit in the network.

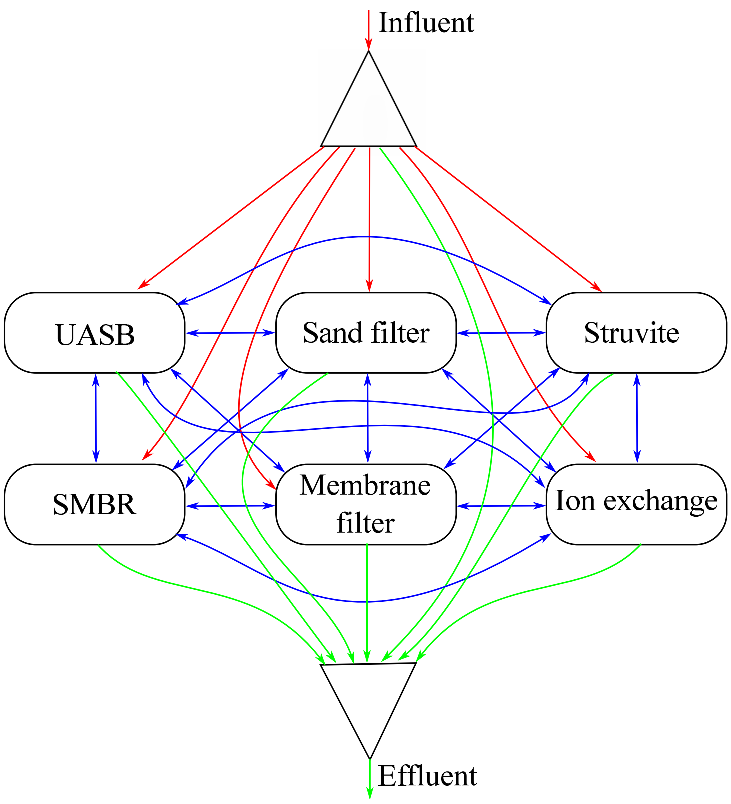



Figure 5.4: Illustration of a simple superstructure layout.

## 5.3 Optimisation Model Formulation

Superstructure-based optimisation is typically formulated as a mixed integer programming (MIP) problem containing two types of decision variables:

- Discrete variables - these are usually binary variables, which decide on the selection of treatment/separation units along with their interconnections to include in the system, here denoted by y; and,

- Continuous variables - this defines the flows and composition as well as certain design and operating parameters, here denoted by x.

An optimisation problem can be posed as the following mathematical programming problem:

$$\begin{aligned} \min_{x,y} \quad & f(x,y) \\ s.t. \quad & h(x) = 0 \\ & g(x,y) \leq 0 \\ & x \geq 0, y \in \{0,1\} \end{aligned} \tag{P}$$

The objective function $f(x, y)$ in (P), which can be expressed as a sustainability, economic, or environmental index is a function of both types of variables. The continuous variables, $x$, which are assumed to be non-negative variables for physical reasons, must follow material balance equations of the form $h(x) = 0$, where usually $\dim(h) < \dim(x)$. Both types of variables also need to satisfy the design specification in terms of discharge allowance, physical operating limits and logical constraints e.g. the existence of unit and piping interconnections for the nonzero flows, or to enforce the sequencing of certain units.

### 5.3.1 Mass Balance

Material balances on flows ($F$) and concentrations ($X$) around the sources, the units, and the sinks are to be obeyed in addition to the discharge limits and certain design and structural specifications as follows: (Note that the sets and indices used in the optimisation formulation are presented in Table 5.1.)

#### 5.3.1.1 Sources

Wastewater influent with contaminants requires further treatment before being discharged into receiving waters. Wastewater can be different types or sources, e.g. municipal, industrial wastewater, or a combination of both. This is sent to the initial splitter to distribute a fraction of the wastewater to other treatment/separation units. Wastewater

Table 5.1: Sets and indices definitions.

| Set | Definition |
|---|---|
| $I$ | set of sources $i$ |
| $J$ | set of sinks $j$ |
| $K$ | set of all treatment units $k$ |
| | where $K = K_{CU} \cup K_{SU} \cup K_{TU} \cup K_{DU} \cup K_{RU}$ |
| $K_{CU}$ | set of primary treatment unit $k$ |
| $K_{SU}$ | set of secondary treatment unit $k$ |
| $K_{TU}$ | set of tertiary treatment unit $k$ |
| $K_{DU}$ | set of sludge treatment unit $k$ |
| $K_{RU}$ | set of recovery unit $k$ |
| $C$ | set of component $c$ |
| $N$ | set of resources recovered from wastewater $n$ |

from sources ($i$) can be sent to treatment units ($k$) and sinks ($j$). In the superstructure-based optimisation approach, it is typically assumed that splitters in the optimisation model are ideal, and concentrations of the outlet streams are equal to the inlet stream. Also, it is possible to have more multiple sources depending on the system under study. The optimiser aims to determine the split fraction of wastewater with given contaminants for subsequent units. The overall mass balances for sources are based on the ideal splitter unit (Figure 5.5), which is given by:

$$F_i^{\text{in}} = \sum_{j \in J} F_{i \longrightarrow j} + \sum_{k \in K} F_{i \longrightarrow k}, \quad \forall i \in I \tag{5.5}$$

where the superscripts $^{\text{in}}$, $^{\text{out}}$ and $^{\text{was}}$ refer to flow/concentrations entering, leaving the unit and sludge produced in the unit, respectively. Each term has corresponding flowrates, while the upper and lower bound constraints are formulated in the form of binary variables to represent the existence of the interconnections between units.

$$yF^{lo} \leq F \leq yF^{up} \tag{5.6}$$

where $F^{lo}$ and $F^{up}$ are the lower and upper bounds of the flowrate; $y$ is the binary variable to define the existence of interconnections, which is equal to zero when the stream does not exist and one in case there is the stream connection.

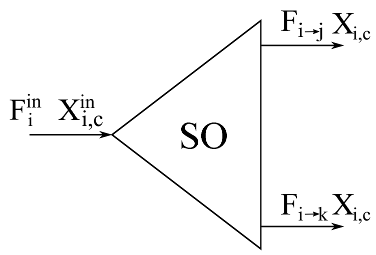



Figure 5.5: Schematic representation of sources.

#### 5.3.1.2 Treatment Units

A group of treatment units is used to remove or recover certain components in the wastewater to satisfy the standard legislation before discharge into the receiving waters. The performance of treatment units are different from one unit to the next, and can be evaluated by means of surrogated models, as mentioned in the previous section. Generally, each treatment/separation unit $k$ is coupled with one mixer (MU) and two splitters (SU1 and SU2) as illustrated in Figure 5.6. Such a combination allows us to consider both wastewater and sludge treatment because some units may produce a portion of sludge, e.g. activated sludge, which needs further treatment before discharge to the environment. Thus, wastewater from some treatment units is splitted into wastewater ($FW$) and sludge ($FS$) streams before being distributed to other treatment units or sinks. For some treatment units, e.g. ion exchangers which do not produce sludge, it is typically assumed that the outlet and inlet flowrates are equal and sludge streams can be neglected from the mass balance equation. Overall, the optimiser aims to select treatment units and interactions among them.

The flows from sources or other treatment units are mixed in the mixer (MU) before sending to the treatment unit $k$. The material balances for each compound $c$ in the mixer can be formulated as follows:

$$\begin{aligned} F_k^{\text{in}} &= \sum_{i \in I} F_{i \longrightarrow k} + \sum_{k' \in K} FW_{k' \longrightarrow k} \\ &+ \sum_{k' \in K} FS_{k' \longrightarrow k}, \quad \forall k, k' \in K,\ k \neq k' \end{aligned} \tag{5.7}$$

$$\begin{aligned} F_k^{\text{in}} X_{k,c}^{\text{in}} &= \sum_{i \in I} F_{i \longrightarrow k} X_{i,c} + \sum_{k' \in K} FW_{k' \longrightarrow k} XW_{k',c} \\ &+ \sum_{k' \in K} FS_{k' \longrightarrow k} XS_{k',c}, \quad \forall k, k' \in K,\ k \neq k' \end{aligned} \tag{5.8}$$

Wastewater from the mixer is then processed by treatment unit $k$. There are typically two outlet streams from the treatment unit: wastewater (FW) and sludge (FS) streams. The flowrate of these streams can be predicted based on the split fraction or the surrogate model, while the outlet concentration can be determined as follow:

$$F_k^{\text{in}} X_{k,c}^{\text{in}} (1 - \rho_{k,c}) = \sum_{k' \in K} FW_{k \longrightarrow k'} XW_{k,c} + \sum_{j \in J} FW_{k \longrightarrow j} XW_{k,c}, \quad \forall k, k' \in K,\ k \neq k' \tag{5.9}$$

$$F_k^{\text{was}} X_{k,c}^{\text{was}} = \sum_{k' \in K} FS_{k \longrightarrow k'} XS_{k,c} + \sum_{j \in J} FS_{k \longrightarrow j} XS_{k,c}, \quad \forall k, k' \in K,\ k \neq k' \tag{5.10}$$

where $\rho_{k,c}$ is the surrogate model developed for the removal performance of a component $c$ in a given treatment/separation unit $k$. Note that $F_k^{\text{in}} X_{k,c}^{\text{in}} (1 - \rho_{k,c})$ or $F_k^{\text{out}} X_{k,c}^{\text{out}}$ and $F_k^{\text{was}} X_{k,c}^{\text{was}}$ can be also replaced by the surrogate model depending on the performance prediction.

#### 5.3.1.3 Sinks

Sinks can be regarded as ideal mixers where wastewater from sources and treatment/ separation units are mixed before discharge into the receiving water (Figure 5.7). Multiple sources and sinks are generally common in the applications of superstructure-based optimisation, e.g. water networks. The optimiser aims to determine the final wastewater effluent with concentrations received from sources and treatment units to satisfy the standard legislation. The material balances for compound $c$ in sink $j$ can be expressed in

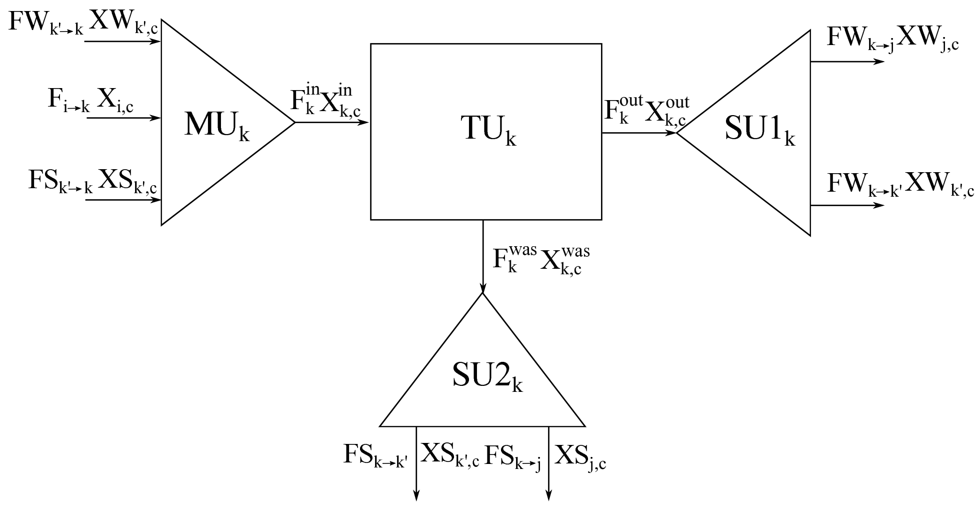



Figure 5.6: Schematic representation of treatment units.

Eq. 5.11 and Eq. 5.12 respectively:

$$F_j^{\text{in}} = \sum_{i \in I} F_{i \longrightarrow j} + \sum_{k \in K} FW_{k \longrightarrow j} + \sum_{k \in K} FS_{k \longrightarrow j}, \quad \forall j \in J \tag{5.11}$$

$$F_j^{\text{in}} X_{j,c}^{\text{in}} = \sum_{i \in I} F_{i \longrightarrow j} X_{i,c} + \sum_{k \in K} FW_{k \longrightarrow j} XW_{k,c} + \sum_{k \in K} FS_{k \longrightarrow j} XS_{k,c}, \quad \forall j \in J \tag{5.12}$$

A constraint is introduced to ensure that compound $c$ present in a given sink $j$ is regulated by the discharge limit $\mathrm{X}_{j,c}^{\max}$ (Eq. 5.13):

$$\sum_{i \in I} F_{i \longrightarrow j} X_{i,c} + \sum_{k \in K} FW_{k \longrightarrow j} XW_{k,c} + \sum_{k \in K} FS_{k \longrightarrow j} XS_{k,c} \leq F_j^{\text{in}} X_{j,c}^{\max}, \quad \forall j \in J \tag{5.13}$$

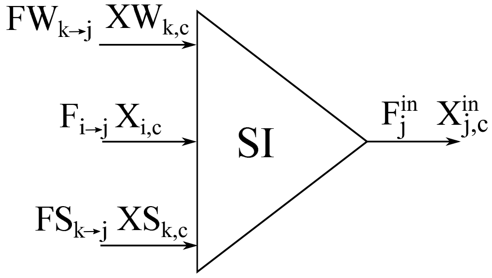



Figure 5.7: Schematic representation of sinks.

### 5.3.2 Objective Function

The optimal system configuration aims to maximise a certain sustainability index of the facility, for instance a weighted sum of LCA impacts [159]. Alternatively, economic efficiency of a facility can be maximised, e.g. life-cycle costing indicator (LCC; [199]) or net present value (NPV) over the project lifetime:

$$\mathrm{NPV} = -\mathrm{CAPEX} + \sum_{y=1}^{\mathrm{LT}} \frac{\text{SALES - OPEX}}{(1+\mathrm{DISC})^{\mathrm{yr}}} \tag{5.14}$$

where LT denotes the project lifetime, typically 20 years; SALES represents revenues from energy/nutrient sales; CAPEX and OPEX denote the costs generated by WWTP capital investment and operation, respectively. DISC is defined as the theoretical rates at which future payoffs are discounted back to present value. The NPV indicates the earning generated by the process/project so the high value (positive) is expected as it can be profitable.

Both CAPEX and OPEX can be predicted using surrogate or approximate models. It is assumed that design parameters i.e. HRT and SRT for all treatment/separation units are fixed so the size can be determined from the the inlet flowrate and selected design parameters. Regarding the surrogate model, it can be simply regressed through a linear function as follow:

$$\mathrm{CAPEX} = \sum_k \mathrm{CAP}_k^{\mathrm{var}} F_k^{in} + y_k \mathrm{CAP}_k^{\mathrm{fix}}, \quad \forall k \in K \tag{5.15}$$

$$\mathrm{OPEX} = \sum_k \mathrm{OP}_k^{\mathrm{var}} F_k^{in} + y_k \mathrm{OP}_k^{\mathrm{fix}}, \quad \forall k \in K \tag{5.16}$$

where $\mathrm{CAP}_k^{\mathrm{var}}$ and $\mathrm{CAP}_k^{\mathrm{fix}}$ are the variable and fixed cost coefficient of CAPEX for a treatment/separation unit $k$; $\mathrm{OP}_k^{\mathrm{var}}$ and $\mathrm{OP}_k^{\mathrm{fix}}$ represent the variable and fixed cost coefficient of OPEX for a treatment/separation unit $k$. These parameters are obtained through the regression of simulated data from the costing software, CapdetWorks®. $F_k^{in}$ and $y_k$ denote the inlet flowrate and the binary variable defining the existence of a treatment unit, $k$. SALES is given by:

$$\mathrm{SALES} = \sum_k \sum_n M^{\mathrm{rec}}_{k,n} \mathrm{PS}_n \mathrm{SD}, \quad \forall k \in K, n \in N \tag{5.17}$$

where $M^{\mathrm{rec}}_{k,n}$ is the amount of resource $n$ recovered in a given treatment unit $k$ calculated using the surrogate model. $\mathrm{PS}_n$ and SD are the price of each resource $n$ and the number of annual operating day.

### 5.3.3 Solution Strategies

The superstructure-based optimisation model leads to a nonconvex MINLP problem due to the presence of bilinear terms which arise in the material balances as a result of composition mixing, in addition to other nonlinearities in the performance and costing equations. Such nonconvexity can lead to multiple local optimal solutions, which require the implementation of global optimisation techniques to guarantee a reliable solution. In this study, the optimisation problem is modeled in GAMS (`http://www.gams.com`), and BARON, which is the deterministic global optimisation solver based on branch and bound algorithms, is used to solve the optimisation problem. To solve nonconvex optimisation problems, it performs convexification of nonconvex functions, e.g. bilinearity, by developing convex and concave envelops as linear under and over estimators. Also, it has special features to enhance the branch and bound approach, including domain reduction and node partitioning schemes. It is good to provide reasonable bounds for the flows and concentrations in the optimisation formulation because they are used for the convex envelops. The global optimisation solver, BARON, has successfully solved superstructure-based optimisation problems with nonconvexity in several applications, especially the synthesis of water network. Recently, Ahmetović and Grossmann [21] and Khor et al. [22] demonstated that BARON is able to solve the well-posed synthesis problems of the water network with multiple water sources, water-using and treatment units and sinks to global optimality. It is worth noting that the proper bounds and logic specifications are used to enhance the solution speed to the global optimum.

In this study, linear logical constraints are applied to the optimisation MINLP model to increase solution speed. Such logical constraints are considered to be the incorporation of qualitative design knowledge based on engineering experience, and design and structure specifications on the interconnections between units and streams can be enforced using these logical constraints. The combination of logical constraints and mixed integer programming in chemical process synthesis has been used for decades. Raman and Grossman [200] proposed using logic constraints in mixed integer programming to represent qualitative and quantitative analysis, respectively. After that these combinations have been implemented in several applications to improve solution convergences, such as in water networks [21, 22].

The logical constraints are able to reduce a number of nonsensical solutions by enforcing restrictions on the values of the binary variables in the branch and bound algorithms; this can reduce the number of nodes, and computational loads. As a result, this increases convergence in solving the optimisation problem by tightening the bounds without eliminating the global optimal solution. The logical constraints used for the synthesis of a wastewater treatment facility are the following:

- Wastewater influent is not allowed to go directly to nutrient recovery units, e.g. ion exchange and struvite precipitation, to prevent suspended solid clogging up the adsorbent. Also, it is not practical for wastewater to be sent to sludge treatment units. This constraint is given by:

$$y_{i \longrightarrow k} = 0, \quad \forall i \in I, \, \forall k \in \{K_{RU} \cup K_{DU}\} \tag{5.18}$$

  where $y_{i \longrightarrow k}$ is the existence of interconnections between the source $i$ and treatment/ separation unit $k$.

- Only one secondary treatment unit (biological treatment) can be selected among a set of biological treatment unit candidates. For example, when the UASB is selected, the SMBR is then neglected. This can be simply expressed as:

$$\sum y_k = 1, \quad \forall k \in K_{SU} \tag{5.19}$$

where $y_k$ is the existence of treatment/separation unit $k$.

- It is practical not to have more than one interconnection between two treatment/separation units:

$$y_{k \longrightarrow k'} + y_{k' \longrightarrow k} \leq 1, \quad \forall k, k' \in K \; k \neq k' \tag{5.20}$$

The model statistics in this case consist of 161 single and 29 binary variables and the computational time is 20 minutes for obtaining the global optimisation based on BARON version 9.0.2

## 5.4 Case study - Industrial wastewater

The synthesis of a resource recovery facility for the treatment of 100 $m^3$/h of an industrial wine distillery effluent was considered here as a case study, and the average composition for the main components in the effluent is given in Table 5.2 [201]. The objective is to maximize the NPV given in Eq. 5.14, while satisfying maximum discharge requirement as defined by the EU Directive 91/271/EEC on Urban Wastewater Treatment. These requirements consist of meeting either minimum reduction of 75% total COD, 80% total N and total P, and 90% TSS or maximum concentrations of 10 g/L total COD, 0.4 g/L total N, 0.07 g/L total P, and 0.5 g/L TSS. The simple superstructure consists of 2 biologi-

Table 5.2: Characteristics of the industrial wine distillery wastewater.

| Total COD | Soluble COD | VFA | TSS | VSS |
|---|---|---|---|---|
| 40 g $L^{-1}$ | 16 g $L^{-1}$ | 48 g $L^{-1}$ | 5 g $L^{-1}$ | 2.8 g $L^{-1}$ |
| Total N | Ammonia | Total P | Phosphates | Alkalinity |
| 2 g $L^{-1}$ | 0.14 g $L^{-1}$ | 0.35 g $L^{-1}$ | 0.16 g $L^{-1}$ | 3100 meq $L^{-1}$ |

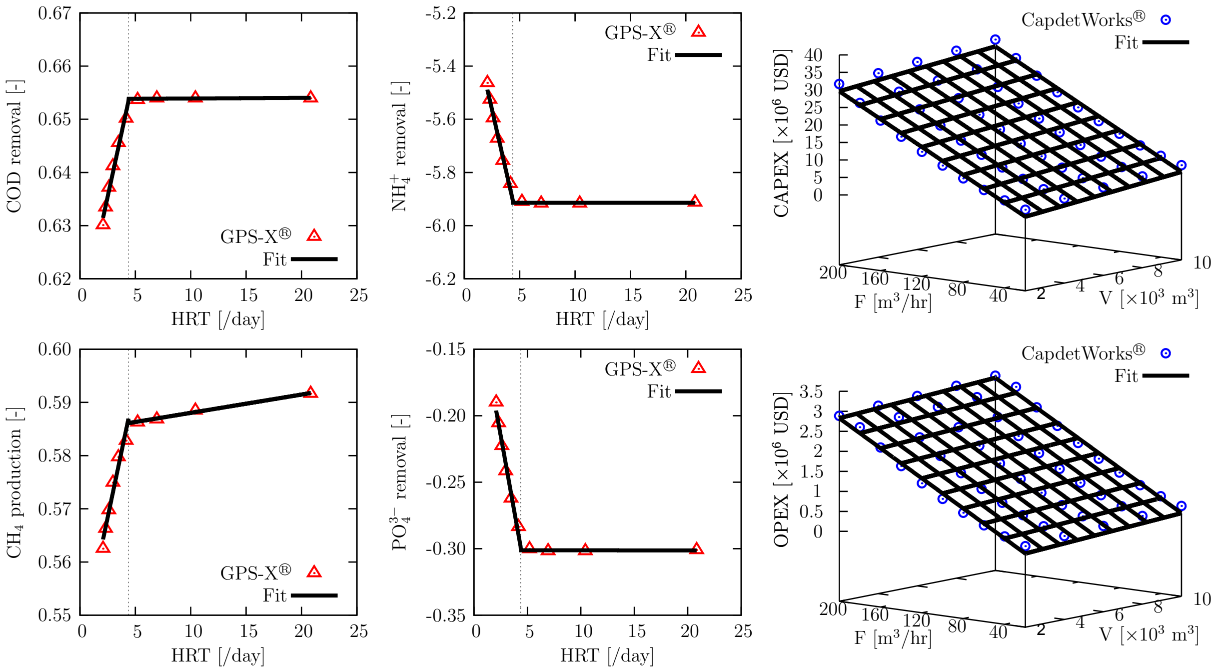



Figure 5.8: Subset of regression models for performance and cost prediction of a UASB unit. Top-left: COD reduction vs. HRT; Bottom-left: COD conversion to CH4 (expressed as equivalent COD) vs. HRT; Top-center: Ammonia reduction vs. HRT (Negative reduction ratios for ammonia and phosphates indicate a net increase due to the conversion of other forms of N and P inside the bioreactor.); Bottom-center: Phosphate reduction vs. HRT (Negative reduction ratios for ammonia and phosphates indicate a net increase due to the conversion of other forms of N and P inside the bioreactor.); Top-right: CAPEX vs. unit volume and influent flow rate; Bottom-right: OPEX vs. unit volume and influent flow rate; Legend: Solid lines represent regression fits; Triangles denote GPS-X® simulation results; Circles denote CapdetWorks® simulation results.

cal treatment units (UASB, SMBR), 2 filtration units (sand filter, membrane unit) and 2 nutrient recovery units (struvite crystallizer, zeolite adsorber) as illustrated by Figure 5.4. This case study is kept relatively simple as the main objective was to assess the proposed optimisation methodology and sludge treatment was not taken into account. More challenging problems which include a variety of treatment/recovery options for carbon, nitrogen and phosphorus as well as sludge treatment will be discussed in the next chapter.

The performance of the UASB and the SMBR are approximated based on the ManTIS2 models in GPS-X®, respectively. The degradation rates of total COD, total N, ammonia, total P, phosphate, and TSS, as well as the production rate of methane in a UASB, are regressed using either linear or piecewise-linear models within an HRT range of 2-20 $d^{-1}$. A subset of these performance models are shown in Figure 5.8 (left and center plots) for a UASB unit. The performance of the filtration, membrane and struvite units is also predicted by using simple models in GPS-X®, and then averaged to yield constant removal/conversion efficiencies as a first approximation. The zeolite (ion exchange) unit, currently unavailable in GPS-X®, is also approximated using constant efficiencies gathered from the literature [202]. The surrogate or the simplified approximate model would be updated iteratively to reduce uncertainty and improve accuracy of model predictions.

The CAPEX and OPEX of all the units, with the exception of the membrane unit, are estimated using CapdetWorks®, and then regressed with simple linear models as a function of the unit volume and/or processed flow rate in the range of operation. This is illustrated in Figure 5.8 (right plots) for the CAPEX and OPEX of a UASB unit. For the membrane unit, currently unavailable in CapdetWorks®, rough estimates of the CAPEX and OPEX were used as recommended by membrane experts [203]. Besides the treatment/separation units in the superstructure, an auxiliary piece of equipment is the electricity generator from biogas. This technology is well developed, with companies such as Alstom, Capston or General Electric providing lines of engines specially adapted for biogas from anaerobic digestion. An average conversion efficiency of 40% is assumed here for the generator, and the OPEX and CAPEX are estimated based on data published by the United Nations Framework Convention on Climate Change (UNFCCC) and the International Energy Agency (IEA);

$$\text{Electricity from biogas} = F_{CH_4} \cdot NCV \cdot \eta \tag{5.21}$$

where $F_{CH_4}$ represents the amount of methane produced in the anaerobic digestion process, $NCV$ is the net calorific value, and $\eta$ is the efficiency of methane conversion to electricity.

An important constraint regarding the interconnections in the superstructure is that the effluent from the UASB cannot pass through the zeolite and/or struvite units directly for nutrient recovery to prevent large concentrations of solids in the recovery units. The optimal configuration is shown at the top of Figure 5.9 - Flowsheet A. Around 60% of the wastewater stream is first split and processed in the UASB unit, before sending it to the sand filter unit together with the remaining 40% of the wastewater influent stream. The outlet stream from the sand filter unit is then sent to the ion exchange column and the struvite crystalizer for nutrient recovery. It turns out that the minimum abatement of 80% in total P is the most restrictive, while the effluent satisfies all other discharge requirements. Additionally, the residual COD concentration is mostly comprised of non-biodegradable soluble compounds, the other part being the biodegradable soluble compounds from the wastewater fraction not treated in the UASB. An NPV of -7.68 M$ was found for the flow-

Table 5.3: Cost analysis for the case study. A: No further restrictions on the interconnections; B: Bypass from source to sand filter not allowed; C: Bypass from source to sand filter or source to sink not allowed.

| Flowsheet | A | B | C |
|---|---|---|---|
| **CAPEX [M$]** | **18.70** | **27.85** | **28.25** |
| UASB (%) | 41.2 | 54.1 | 54.2 |
| Electicity generator (%) | 14.4 | 16.4 | 16.4 |
| Sand filter (%) | 14.1 | 9.4 | 9.3 |
| Struvite crystalizer (%) | 13.2 | 8.8 | 8.8 |
| Ion exchange column (%) | 17.1 | 11.3 | 11.3 |
| | | | |
| **OPEX [M$/year]** | **1.69** | **2.78** | **2.86** |
| UASB (%) | 41.2 | 54.1 | 54.2 |
| Electricity generator (%) | 14.4 | 16.4 | 16.4 |
| Sand filter (%) | 14.1 | 9.4 | 9.3 |
| Struvite crystalizer (%) | 13.2 | 8.8 | 8.8 |
| Ion exchange column (%) | 17.1 | 11.3 | 11.3 |
| | | | |
| **SALES [M$/year]** | **2.57** | **4.19** | **4.25** |
| Electrical power (%) | 80.4 | 83.5 | 83.5 |
| Struvite fertilizer (%) | 6.2 | 4.0 | 4.0 |
| Ammonia (%) | 13.4 | 12.5 | 12.5 |
| | | | |
| **NPV [M$]** | **7.68** | **10.75** | **10.93** |

sheet A over a period of 20 years (an increase/decrease in a period of time would slightly affect the NPV due to the fact that it is dominated by CAPEX.), and the breakdown of these costs in terms of CAPEX, OPEX and SALES is shown in Table 5.3. The large CAPEX, of which more than 40% is accounted for by the UASB unit, cannot be offset by the net annual profit of about 0.88 M$, even though, the sales revenue, mainly electricity from biogas combustion, is more than the OPEX., and this leads to the negative NPV. Although a resource recovery facility may not completely offset the infrastructure and operating costs solely based on electricity and nutrient sales, it would be great to mitigate the cost of wastewater treatment to complying with the discharge regulations. The

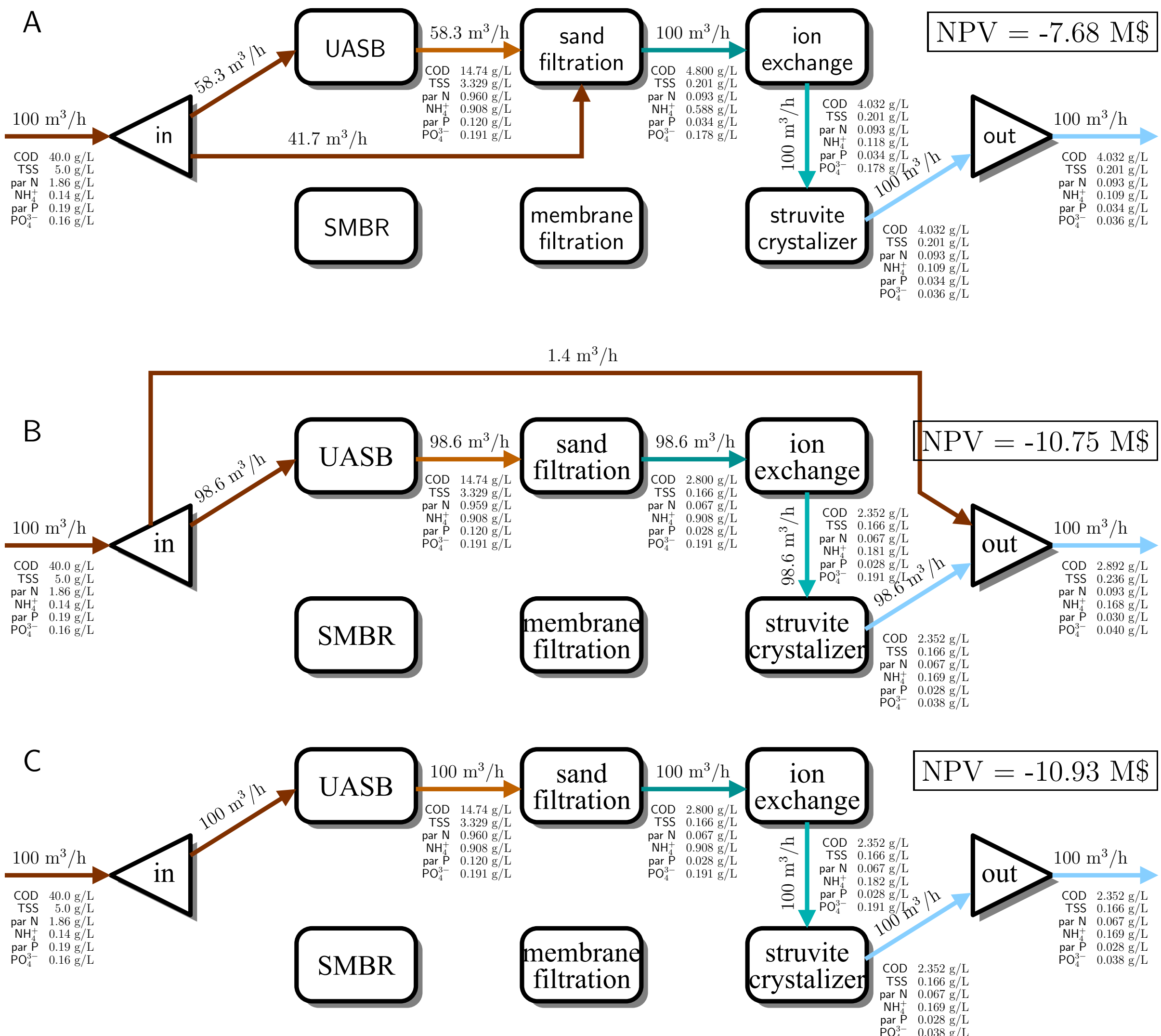



Figure 5.9: Optimal superstructures for the case study A: No further restrictions on the interconnections; B: Bypass from source to sand filter not allowed; C: Bypass from source to sand filter or source to sink not allowed.

decision to split the wastewater stream and divert around 40% of that stream around the UASB , which is then not processed, may first appear to be counter-intuitive given the fact that most of the sales revenue is from the biogas produced in the UASB. However, producing more biogas is only justified in terms of the NPV when the added sales revenue can offset the extra CAPEX and OPEX for a larger UASB unit. Such a condition is not met in this case study, and it is worth investigating the sensivity of this trade-off further to validate this conclusion.

To confirm this assumption, the possibility of bypassing the UASB by sending part of the wastewater stream directly to the filtration units was removed; the optimal superstructure is depicted in Figure 5.9 - Flowsheet B. In this flowsheet, a small fraction of the wastewater stream is now sent directly to mix with the treated effluent stream without being processed by treatment/separation units. Expectedly, the estimated NPV value of Flowsheet B decreases in comparison with Flowsheet A- see Table 5.3 for the breakdown cost. In particular, there is a large reduction of around 3 M$. Finally, when a small fraction of the wastewater stream is not allowed to be sent directly to mix with the treated effluent, this can lead to the optimal superstructure depicted in Figure 5.9- Flowsheet C. The estimated NPV of this flowsheet turns out to be comparable with the estimated NPV of Flowsheet B.

## 5.5 Summary

In this chapter, a systematic optimisation-based methodology for the synthesis of wastewater/resource recovery facilities has been discussed and illustrated with a case study. By and large, this methodology should be regarded as a decision support system for isolating, among hundreds or even thousands of alternatives, those promising resource recovery systems whose development is worth pursuing. Based on this pre-selection, further simulation and optimisation studies can then be undertaken to refine the performance and cost predictions by taking into account detailed design and operation considerations, as well as process integration. Such decomposition is indeed warranted as current computational capabilities and available algorithms do not allow for the optimal design and operation to be solved in a single step due to complex unit configuration, multiple scales, time dependence, and uncertainty.

A major hurdle in applying this methodology appears to be the availability of reliable performance models for the treatment and separation units, as well as reliable (capital and operation) costing data. Here, we advocate the use of state-of-the-art wastewater treatment simulators in order to derive simple response-surface models, which are general enough to be independent of detailed design choices and keep the superstructure optimisation model computationally tractable-this approach was demonstrated in a simple case study. Naturally, such simple models carry significant uncertainty and usually only provide a rough approximation of the actual performance of such complex units. A way to refine these models involves performing an iteration between the detailed process simulators and the superstructure optimisation problem. Moreover, for those treatment/recovery techniques that are less well established, or lack reliable performance models, a scenario based analysis can be applied, whereby multiple sets of resource recovery systems are determined on account of the forecast performance and cost scenarios. In particular, this analysis can be useful for resource allocation, for instance to help determine which technologies are critical and on which to focus further research and development efforts.

# Chapter 6

# Synthesis of Wastewater Recovery Facilities using Enviroeconomic Optimisation

## 6.1 Introduction

Wastewater treatment processes are considered as end-of-pipe technologies to handle environmental issues concerned with wastewater discharges, and minimise the environmental impacts of pollutants discharged into a water body. Also, environmental authorities concerned with wastewater treatment are likely to adopt stricter wastewater standards to protect receiving waters. On balance, this may have negative impacts on the environment due to the increased emissions of GHGs, e.g. global climate change. Most studies investigate a variety of approaches to reducing a particular pollutant in the process, or focus on economic aspects, with little attention paid to a wide range of environmental issues. Nevertheless, while this approach has led to substantial improvements in economic and environmental impacts, the scope of most of these studies is still limited. Some provided solutions that could efficiently reduce one environmental impact, but shift the problem to another sphere of concern, e.g. global warming. Hence unless there is an integrated approach, problem-shifting occurs which cannot provide holistic and sufficient solutions for decision-makers. Given the need for sustainability, the main objective of wastewater treatment should go beyond the environmental impact on surface waters, and the protection of human health [204]. Recently, considerable research attention has been paid to the application of life cycle assessment (LCA) to wastewater treatment processes [159, 205, 206]. LCA is a holistic method which considers all of the processes over an entire life cycle, including input (e.g. input energy) and output (e.g. waste and emissions) flows. The analysis is based on cradle-to-grave that covers all activities from raw material acquisition, manufacture, use of product and its end-of-life. The incorporation of the LCA into the unified framework has been advocated by recent optimisation techniques and application, and has lead to the concept of multi-objective optimisation where two or more conflicting objectives are optimised.

This chapter is concerned with extending the methodology presented in the previous Chapter by incorporating LCA into the decision-making process in order to promote sustainable WWTP designs, alongside economic viability. The remainder of the Chapter is organised as follows: Section 6.2 presents the general concepts of LCA and multi-objective optimisation, including a review of recent work on synthesis problems incorporating LCA. Section 6.3 focuses on the development of environmental performance indicators based on the LCA approach and case study definition, while solution strategies to handle the multi-objective optimisation problem are discussed in Section 6.3.2. The results of a case study with the synthesis of municipal wastewater treatment facility based on the proposed approach is presented in Section 6.4.

# 6.2 Background

## 6.2.1 LCA

LCA is a methodology to quantify the environmental impacts with respect to products, services and processes throughout their life cycle from cradle-to-grave. It accounts for every stage of a product/process, from raw materials acquisition to final disposal. LCA has been widely recognised as a decision-making tool for identifying the "hot spots", i.e. the main contributors to environmental issues. The LCA framework has been formalised in a series of International Standards (ISO 14040) [207], consisting of four stages: goal and scope definition, inventory analysis, impact assessment and interpretation (Figure 6.1). The details of the LCA methodology is provided as follows:

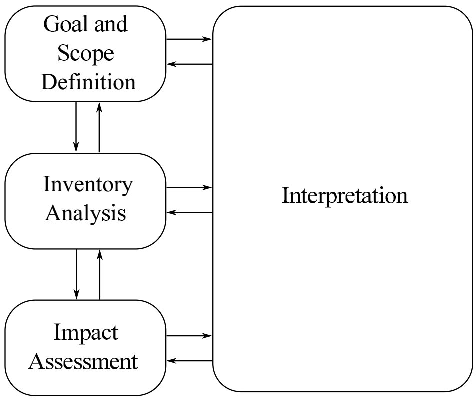



Figure 6.1: Phases of an LCA [207].

### 6.2.1.1 Goal and scope definition

The study goals and scope are defined in this phase. This includes the rational for the investigation, intended applications and audience, system boundaries, the functional unit (the important basis on which processes or products can be compared), allocation methodology, data requirements, impact categories and impact assessment approach (characterization, normalization).

#### 6.2.1.2 Inventory analysis

This phase involves a compilation of the input/output of the processes/products over their life cycles. The relevant materials, energy flows and emissions throughout the different stages of the process or product life cycle are quantified to provide the inputs and outputs associated with the process or product. The inventory data can be obtained from lab, industrial operation, and estimation from experts, model predictions, relevant literature and LCA databases. This data is then used to calculate the set of environmental impacts of the process in the next phase. Therefore, the analysis depends on the quantities and types of materials and energy used during its lifespan.

#### 6.2.1.3 Impact assessment

This phase aims to classify and link the input-output flows to relevant environmental aspects, and evaluate the potential environmental impacts of the whole process or system based on the results from the inventory analysis [207]. It consists of compulsory (classification and characterization) and optional (normalization and weighting) activities. Classification and characterization stages involve the transformation of data from the inventory analysis which corresponds to inputs and outputs of materials, energy and emissions into impact indicators. Initially, the impact categories are defined and selected to describe the impacts caused by the process or product during production, use and disposal. There are two approaches developed to describe the pathway from the inventory analysis to the environmental impacts: midpoint and endpoint approaches. The mid-point approach is known as the problem-oriented approach; it is the impact indicator which represents the mid pathway of impacts before the endpoint. Real phenomena such as global warming potential, acidification and eutrophication can be translated from the midpoint impact category. The other approach is the endpoint, also known as the damage-oriented approach. This refers to the impact indicator for each impact category at the end of the impact pathway based on the area of protection, e.g. human health, ecosystem quality and natural resources [208]. Figure 6.2 illustrates the environmental impact assessment mechanism describing transformation of a substance into a series of impacts which eventually leads to damages to the environmental areas of protection. Also, the difference between the midpoint and endpoint considerations along the pathways mechanisms is shown. After the selection of impact catagories, the contribution of each input and output to the environment is mapped into these impact catagories and impact indicators, corresponding to the potential impacts on the environment. Having obtained this data, it is then optional to perform normalization and weighting. Normalization enables us to compare all the environmental impacts on the same scale where the factors are obtained from regional and global databases. One way to carry out normalization is to divide each impact indicator by the difference between the maximum and minimum values, which scales all impact indicators into a range between zero and one [209]. Finally, the different environmental impact catagories are grouped or weighted to convert or aggregate environmental indicators categories into one single indicator. It is important to apply different weighting factors to investigate their effects on trade-offs between different impact indicators. The weighting factors can be defined by the experts or using other techniques, e.g. monetarization to facilitate the interpretation of the system [210].

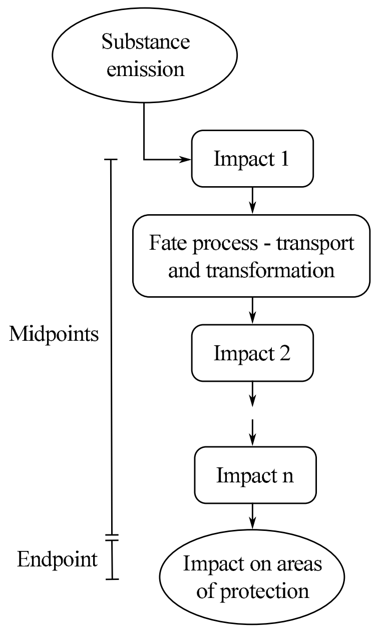



Figure 6.2: Schematic representation of the difference between midpoint and endpoint impact assessment [211].

#### 6.2.1.4 Interpretation

The results from the impact assessment are interpreted for the decision-making process. The critical environmental concerns, and the significant contribution of a certain process or product to the environment can be identified. It is suggested to verify the results by evaluating the consistency of the approaches, or perform data quality analysis (including sensitivity and uncertainty analyses) to improve the degree of confidence resulting from uncertainties in the data or the selected approaches. Although LCA is a powerful tool to evaluate the environmental impacts, it is evident that data quality and collection is the main limitation of the LCA method. The LCA methodology is dependent to data so the availability and quality would affect the overall quality of LCA results. Data selection and analysis needs to be performed to improve accuracy and quality of the results [212].

### 6.2.2 Applications of LCA in Process Design

Traditionally, researchers in the process system engineering (PSE) community apply optimisation models to design chemical processes and assist in their operation, which focuses on maximisation of a given economic performance while satisfying mass balances and capacity constraints. However, awareness of the need to integrate environmental concerns into economical criteria has been growing steadily in the past decade. This trend has been motivated by several issues, but primarily from the government and regulatory policy to tighten environmental regulations [213]. LCA has been used as a decision-making tool to assess the environmental impacts of several applications in process design to improve environmental performance [214, 215]. Over the past decade, several attempts have been made to incorporate the environmental impacts into the optimisation model to satisfy environmental, economic and social goals simultaneously.

Stefanis et al. [216] developed a methodology to include LCA into a process optimisation framework, and involved the definition of process boundaries, analyses of data inventory and quantification of environmental impacts. In this case, all environmental impacts were added in terms of the global environmental impacts which could be incorporated as environmental criteria in process optimisation. Later, Azapegic and Clift [214] proposed the use of multi-objective optimisation to simultaneously optimise a number of environmental objectives, quantified by means of the LCA approach. Previous research also demonstrated that it is possible to achieve a trade-off between environmental and economic performance. Hugo and Pistikopoulos [217] presented a mathematical programming approach for incorporating LCA into the strategic investment of supply chain networks. Their design involved the selection, allocation, and capacity expansion of processing technologies and transportation links to satisfy the demands. Such an approach could be formulated as a multi-objective mixed integer linear programming problem (mo-MILP), which can be applied as a decision-making tool for strategic investment planning allowing for environmental impacts. Guillén et al. [213] proposed a similar framework for chemical process design incorporating environmental evaluation by means of the LCA. The conceptual design is based on the superstructure optimisation of sustainable chemical process which is formulated as a mixed-integer problem. The LCA is assessed by the Eco-indicator-99, reflecting the environmental problems at damage level. The addition of an environmental indicator can lead to multi-objective optimisation, where the trade-off solutions exist between cost and environmental impact, and the case study was the design of the hydrodealkylation (HDA) of toluene. The results show that environmental improvements in the process are possible through structural modifications and operational changes. Also, a framework for process design coupled with the environmental impact can provide insights into the design problem, and can be considered as a decision-making tool to provide more sustainable alternatives.

More specifically in the design of WWTPs, the LCA approach was first applied in the 1990s to evaluate different small-scale wastewater treatment technologies [218]. Some studies have applied LCA to plant operation, excluding the design and development phase, because it is normally assumed that this phase does not contribute much to the environment impact of a WWTP. However, it turns out that the design and development phase can influence the environmental impacts in the other phases [219]. For example, design of wastewater treatment affects the amount of energy consumption required and emissions in for the operation phase. Various LCA studies have been carried out to compare different treatment technologies in wastewater treatment systems [220, 206, 221] or sludge management technologies [222], and for evaluating the main environmental impacts associated to specific wastewater treatment processes [223, 204]. Sensitivity of the LCA results to various impact assessment methods has also been investigated [205]. However, these studies have a number of limitations in terms of the limited number of process alternatives or configurations investigated, the size of the process, and the exclusion of some aspects of WWTPs, especially the exclusion of sludge treatment [206]. Also, such comparative LCA studies of different wastewater treatment technologies only provide partial and insufficient information for decision makers. As pointed out in the recent review paper by Corominas et al. [159], however, there is a need for better linking LCA with economic and societal assessments in order to provide a more complete and accurate sustainability picture to decision makers. The combination of LCA methodology and other criteria i.e. economical aspects can be a powerful decision-making tool and provide valuable insights to achieve sustainability. Recently, Garrido-Baserba et al. [224] have incorporated LCA evaluation into a knowledge-based decision-support system to design wastewater treatment plants (WWTPs). The results demonstrate the potential of LCA for decision making, although the approach is largely dependent on the data quality and their specifications [225]. Moreover, this approach may not provide further information with regards to the optimal (or near-optimal) solutions.

### 6.2.3 Multi-objective Optimisation

Multi-objective optimisation (MOO) refers to the optimisation of two or more conflicting objectives. Most engineering problems have multiple objective e.g. maximise profit, minimise environmental impacts. For multi-objective optimisation, the best compromise solutions for all objective functions are determined. Note that it is impossible to improve one objective without deteriorating the other objectives, and this is known as Pareto optimality [213]. The main advantage of multi-objective optimisation is a set of Pareto-optimal solutions representing the compromise between the criteria considered is generated instead of one solution and this allows decision-makers to further explore trade-offs. Note that a set of Pareto optimal solutions is typically called the Pareto front. A good Pareto frontier should be evenly distributed and cover a wide range of objective values under study, and can be convex, concave or both, and contain discontinuities. A convex Pareto frontier is better than a concave one, and it is common to have the Pareto frontier with discontinuities for engineering applications, which are complex [226].

Several approaches have been developed to solve the multi-objective optimisation problems to find the Pareto-optimal solutions. This includes weighted, $\varepsilon$-constraints, goal programming, meta-heuristic/stochastic approaches, which can be grouped in different ways depending on preference of decision makers, i.e. priori, posteriori and without preferences or one and many solutions obtained in one run [226]. Evolutionary algorithm, e.g. non-dominated sorting genetic algorithm (NSGA) is another approach that is suitable for solving multi-objective optimisation which allows to compute the entire Pareto front but the shortcoming of this approach is related to the lower speed and the global optimal solution is not guaranteed [227]. Different approaches have their own advantages and disadvantages for solving these problems, however, the $\varepsilon$-constraints approach will become the main focus of this study because it is a promising approach among alternatives, and has already been applied in several studies on engineering applications [213, 217]. The multi-objective optimisation is transformed into a single objective optimisation problem, which can be solved by global deterministic solvers, and is the main focus in this work. The Pareto frontier can be found by changing the preference or constraints, but nevertheless, this requires more than one run to generate a set of Pareto solutions.

In the field of wastewater treatment, conflicting objectives such as effluent quality and energy consumption are typically found; to improve effluent quality typically requires more energy use. Traditionally, these problems have been addressed using single objective optimisation through weighting of the various contributions in an overall cost index. However, multi-objective optimisation has been mostly applied to the operation phase, especially the implementation of automatic control to investigate the effects of different control strategies, and to balance the trade-offs between GHG emissions, effluent quality and operational cost [228, 229, 230]. Multi-objective optimisation has not been applied widely in WWTP design to date, perhaps due to the complexity of wastewater treatment processes. Flores-Alsina et al. [231] have proposed a decision-making tool to support the design of WWTPs based on multi-criteria evaluation. The selection of different process alternatives is based on an overall degree-of-satisfaction index, as obtained through the weighting of selected criteria and objectives, and it relies on a mix of mathematical modeling and qualitative knowledge. Hakanen et al. [232] have presented an interactive multi-objective optimisation platform coupled with model-based simulation, called NIMBUS. This platform allows a decision maker to simultaneously consider the design of WWTPs from different standpoints and to balance between the different objectives. More recently, Bisinella-de-Faria et al. [233] have developed an integrated framework combining LCA with dynamic simulation to compare different treatment processes, with a focus on source separation and energy/nutrient recovery. On the whole, these existing approaches are certainly heading in the right direction, but the exploration remains limited to a small number of process configurations nonetheless. In contrast, the following section presents and illustrates a superstructure modeling and optimisation approach, which may resolve some of these limitations.

## 6.3 Enviroeconomic Optimisation Methodology

As the general methodology framework is described and illustrated by the simple case study in the previous chapter, here we will focus on incorporation of LCA methodology into the unified optimisation framework and evaluation of environmental impact assessment to achieve economic and environmental sustainability. The synthesis of wastewater treatment facilities incorporating environmental impacts leads to multi-objective mixed integer nonlinear programming (MO-MINLP) as follows:

$$\begin{aligned} \min_{x,y} \quad & [KPI_1(x,y), KPI_2(x,y), ...] \\ s.t. \quad & h(x) = 0 \\ & g(x,y) \leq 0 \\ & x \in R^n, y \in \{0,1\}^m \end{aligned} \tag{Q}$$

The objective of the MO-MINLP consists of minimising two or more key performance indicators (KPIs), which are functions of both continuous and discrete variables. Again, these variables must satisfy restrictions of the form $g(x, y) < 0$ , either design specifications in terms of discharge allowance and physical operating limits, or logical constraints for the existence of piping interconnections with nonzero flows or the sequencing of certain units. Last, but not least importantly, the continuous variables $x$ must obey material balance equations of the form $h(x) = 0$ (see Section 5.3.1), where usually $\dim(h) < \dim(x)$, describing models of the physical units. Regarding the objective functions or KPIs, here multiple conflicting objectives are considered. One is the net present value (NPV) which considers both CAPEX and OPEX of the wastewater treatment facilities (see Section 5.3.2). The other objectives are regarded as environmental impacts and the following section presents an approach to develop such environmental performance indicators.

### 6.3.1 Environmental Impact Assessment

The LCA principles are applied to evaluate the design alternatives from the environmental viewpoint. As a result, these impacts can be used as a decision criterion to select those process alternatives with improved environmental performance. The methodology for incorporating environmental performance indicators follows the four phases of LCA.

#### 6.3.1.1 Goal and scope definition

The main goal of this study was to incorporate LCA into a systematic optimisation framework. With respect to the system boundaries, we consider the entire life cycle of wastewater treatment processes ranging from design (infrastructure) and operation (energy consumption and emissions) to reduce overall environmental impacts. The analysis covers all steps of the wastewater treatment processes, ranging from the wastewater influent to effluent including sludge treatment produced as a by-product in the process. In addition, the construction, operation and emissions are accounted for a certain period of time. Figure 6.4 shows the system boundary for the wastewater treatment facility, including sludge treatment processes under study. With regards to the functional unit, it was chosen based on different objectives under study. The functional unit in this work was based on a given fixed amount of wastewater influent (volume of wastewater within a period of time) because it is clear and easy to establish an inventory [234].

#### 6.3.1.2 Inventory analysis

The main objective of this phase is to quantify the material and energy inputs and outputs associated with the process, where all stages in the system boundaries are included, and then a set of environmental impacts can be determined. In this study, the selected elements for inventory data are presented in Table 6.1. Data for the inputs and outputs of the material and energy balance, including the main sources of environmental burdens, e.g. construction materials (concrete and steel), effluent quality (COD, $NH_4^+$-N), sludge production and direct emissions were obtained from the modeling approach. However, models for wastewater treatment processes, especially biological wastewater treatment, are complex and it is computationally intractable for global optimisation to combine these models into the optimisation framework. The proposed approach to handle this problem was to develop a simple, yet reliable, model or surrogate model (or approximate model as defined in the previous Chapter) to generate a set of inputs and outputs of the materials and energy associated with the process. Such a surrogate model was developed based on data obtained from the simulation data of individual treatment/ separation process by using the commercial wastewater treatment process simulator GPS-X®.

Table 6.1: Selected elements for wastewater treatment inventory.

| Parameter | Unit |
|---|---|
| Energy use | |
| Electricity from grid | kWh |
| Direct emissions | |
| $N_2O$ to air | $tCO_2$ |
| $CO_2$ to air | $tCO_2$ |
| $CH_4$ to air | $tCO_2$ |
| Avoided products | |
| Mg as fertiliser | kg |
| N as fertiliser | kg |
| $P_2O_5$as fertiliser | kg |
| $NH_4^+$-N | kg |
| Electricity from CHP | kWh |
| Construction materials | |
| Concrete | Tons |
| Steel | Tons |
| Wastewater & sludge | |
| COD to water | kg |
| TSS to water | kg |
| $NH_4^+$-N to water | kg |
| $NO_3^-$-N to water | kg |
| $PO_4^{3-}$-P to water | kg |

#### 6.3.1.3 Impact assessment

In this phase, data from the inventory analysis was translated into the corresponding environmental impact using standard parameter values available in the environmental databases. A problem-oriented (mid-point) approach CML2 baseline 2000 is used as the life cycle assessment (LCIA) method. Initially, we consider two impact catagories, which are commonly used to evaluate the environmental impacts in the field of wastewater treatment [159] (more impact catagories can be included in a future study, e.g. acidification.); a description of two environmental impact indicators is presented in Table 6.2. These two impact indicators are combined with the economic objective (NPV), and are incorporated into the optimisation problems as key performance indicators. The overall load for a given

Table 6.2: Selected impact catagory and its description under study.

| Impact Category | Description |
|---|---|
| Global warming potential (GWP) | The overall and potential climate change associated with GHGs emissions, and has the same effect as $CO_2$ in reflecting heat radiation. GWP is quantified based on the cumulative radiative forcing impacts of a particular greenhouse gas over a period of time. |
| Eutrophication | The enrichment of nutrients in aquatic and terrestrial ecosystems leading to an increase in the production of algae, phytoplankton and/or higher aquatic plants. This can reduce the amount of oxygen dissolved in water and lead to a deterioration in water quality. |

category $l$ can be quantified as follows (Eq.6.1).

$$\mathrm{KPI}_l = \mathrm{INFRA}_l + \mathrm{LT} \cdot (\mathrm{OPER}_l + \mathrm{WWEFF}_l + \mathrm{WWSLU}_l - \mathrm{CRED}_l) \tag{6.1}$$

where $\mathrm{INFRA}_l$, $\mathrm{OPER}_l$, $\mathrm{WWEFF}_l$, $\mathrm{WWSLU}_l$ and $\mathrm{CRED}_l$ represent the individual loads associated with the required infrastructure, annual operation of the plant, discharged effluent, discharged sludge, and obtained credit, respectively. All these loads may themselves be computed as combinations of a list of 'elementary' environmental burdens corresponding – but not limited – to: the use of steel, concrete or electrical power; the emissions of $CO_2$ or methane from the treatment units; the release of COD, ammonia, phosphates or suspended solids with the treated effluent; and the utilization of nitrogen, phosphorus or magnesium resources. In particular, these elementary impacts can be obtained from the EcoInvent data base, which is available through LCA software such as SimaPro® as presented in Table 6.3. Aggregation of these various burdens into the loads in Eq. (6.1) relies on inventory data predicted by the performance surrogates. The environmental impacts from each individual load were selected as follows here:

- Inventory data for both wastewater and sludge streams was simply obtained through the simulation/optimisation of the wastewater treatment facility. The loads of wastewater ($\mathrm{WWEFF}_l$) and sludge ($\mathrm{WWSLU}_l$) discharge to the environment can

Table 6.3: Charactersation factors of selected elements for two impact catagories under study.

| Parameter | Unit | Eutrophication, kg $PO_4^{3-}$/unit | GWP100, kg $CO_2$e/unit |
|---|---|---|---|
| Electricity from grid | kWh | 7.34E-3 | 0.47 |
| $N_2O$ to air | kg | - | 298 |
| $CO_2$ to air | kg | - | 1 |
| $CH_4$ to air | kg | - | 25 |
| Mg as fertiliser | kg | 1.8E-3 | 1.77 |
| N as fertiliser | kg | 5.94E-3 | 7.04 |
| $P_2O_5$as fertiliser | kg | 3.08E-2 | 1.2 |
| N as ammonium nitrate | kg | 6.8E-3 | 8.54 |
| Concrete | kg | 0.11 | 0.44 |
| Steel | kg | 24.95 | 39.99 |
| COD to water | kg | 2.20E-02 | - |
| $NH_4^+$-N to water | kg | 0.33 | - |
| $NO_3^-$-N to water | kg | 0.1 | - |
| $PO_4^{3-}$-P to water | kg | 1 | - |

be determined as follows:

$$\mathrm{WWEFF}_l = \sum_v \alpha_{l,v} \mathrm{EFF}_v \mathrm{SD} \tag{6.2}$$

$$\mathrm{WWSLU}_l. = \sum_v \alpha_{l,v} \mathrm{SLU}_v \mathrm{SD} \tag{6.3}$$

where EFF, SLU denote the amount of wastewater effluent and discharged sludged for a given element $v$; SD is the number of annual production days and $\alpha_{l,v}$ is the characterization factor of a given element $v$ for the impact catagory $l$.

- The amount of construction materials (e.g. concrete, steel) required to contstruct wastewater treatment facilities was predicted by means of costing software such as CapdetWorks® based on selected design parameters (e.g. HRT, SRT). As a first approximation, the loads may be assumed to scale linearly with the inventory flows.

$$\mathrm{INFRA}_l = \sum_k \sum_{\mathrm{v}} \alpha_{l,v} (\mathrm{INF}^{\mathrm{var}}_{k,v} F^{\mathrm{in}}_k + y_k \mathrm{INF}^{\mathrm{fix}}_{k,v}) \tag{6.4}$$

where $\mathrm{INF}^{\mathrm{var}}_{k,v}$ and $\mathrm{INF}^{\mathrm{fix}}_{k,v}$ denote variable and constant terms for the infrastructure material $v$ of the unit $k$. $F^{\mathrm{in}}_k$ is the wastewater influent of the unit $k$ and $y_k$ is the binary variable to define the existence of the unit $k$. Note that all constant and variable terms used for the predictions of environmental impacts can be obtained by the regression model.

- The environmental impact associated with operation includes electricity, emissions from biogas combustion, direct emission, e.g. $N_2O$, $CH_4$, $CO_2$ from biological treatment. The inventory data for this group was calculated using the new wastewater treatment model, ManTIS3 available in GPS-X® and costing software CapdetWorks®. Then, the loads from operation based on the surrogate model were given by.

$$\begin{aligned}\mathrm{OPER}_l = \sum_k \sum_v \alpha_{l,v} [(\mathrm{OPE}^{\mathrm{var}}_{k,v} F^{\mathrm{in}}_k + y_k \mathrm{OPE}^{\mathrm{fix}}_{k,v}) + F^{\mathrm{CO_2}}_k \rho_{\mathrm{CO_2}} \mathrm{SD} \\ + F^{\mathrm{in}}_k (\mathrm{CARB}^{\mathrm{var}}_{k,v} X^{\mathrm{in}}_{k,v} + \mathrm{CARB}^{\mathrm{fix}}_{k,v})] \end{aligned} \quad (6.5)$$

where $\mathrm{OPE}^{\mathrm{var}}_{k,v}$ and $\mathrm{OPE}^{\mathrm{fix}}_{k,v}$ denote the projected variable and constant terms of operational input/output $v$ for unit $k$ including electricity. $F^{\mathrm{CO_2}}_k$ and $\rho_{\mathrm{CO_2}}$ are the flowrate of $CO_2$ from biogas combustion produced by the unit $k$ and density of $CO_2$.

- In order to account for credits of recovering resources from wastewater, electricity produced from biogas, struvite and ammonia were considered. The amount of resources were calculated based on performance of each treatment/separation unit predicted by the process simulator or data in the literature (for ion-exchanger).

$$\mathrm{CRED}_l = \sum_k \sum_v \alpha_{l,v} M^{\mathrm{rec}}_{k,v} \mathrm{SD} \quad (6.6)$$

where $M^{\mathrm{rec}}_{k,v}$ is amount of resource $v$ recovered from the unit $k$.

#### 6.3.1.4 Interpretation

The results obtained from the optimisation were analyzed, and include conclusions and a recommendation for the formulated system. Note that this approach can provide insight into the synthesis problem which enables us to find the trade-off between the objectives. The results obtained from the multi-objective optimisation should lie on the Pareto-frontier.

### 6.3.2 Numerical Solution Strategies

A challenging task for WWTP design apart from nonconvexity discussed in Section 5.3.3 is to satisfy multiple conflicting objectives simultaneously, while meeting the discharge regulations. As mentioned in the previous section, there are several approaches proposed to handle these multi-objective optimisation problems. One of the most widely used in process engineering is the $\varepsilon_i$-constraints, which is based on the conversion of multiple-objectives into a single objective optimisation problem. This approach was first introduced by Haimes et al. [235] to generate a set of solutions. The concept of this approach is to maximise one of the objective functions and convert the other objectives into constraints bounded by the allowable levels, which can be modified to generate the complete Pareto optimal frontier:

$$\begin{aligned} \min_{x,y} \quad & KPI_1(x,y) \\ s.t. \quad & KPI_i(x,y) \leq \varepsilon_i \quad i = 2, 3.., n_f \\ & h(x) = 0 \\ & g(x,y) \leq 0 \\ & x \in R^n, y \in \{0,1\}^m \end{aligned} \tag{R}$$

where $n_f$ is the number of key performance indicators. The set of Pareto solutions to the original multi-objective optimisation problem can be obtained from solving the problem for all possible $\varepsilon_i$.

An illustration of the Pareto frontier is depicted in Figure 6.3; here we consider two objective functions: economic, and environmental impact. The optimal solutions of the problem are the points that lie on the Pareto curve, and it is worth noting that there is no solution below the curve due to a violation of Pareto optimality. The decision maker is likely to choose from the set of Pareto solutions which optimise particular preferences, while the other objectives are still satisfied at the same time. Note that the formulated optimisation problem is non-convex due to the presence of bilinearity, and a global optimisation solver is required to compute the Pareto frontier, which is discussed in the previous chapter. Note that the optimisation model in this study consists of 407 single and 90 binary variables. The computational time ranges from 30 minutes to 7 days depending on the objective function and constraints based on BARON version 12.7.7.

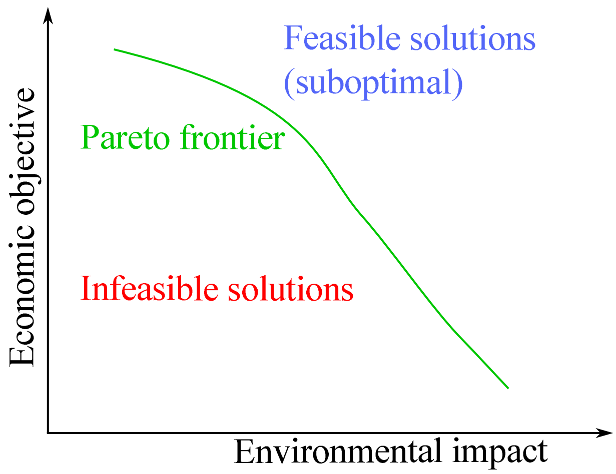



Figure 6.3: Illustration of a Pareto curve.

## 6.4 Case Study - Municipal Wastewater with Biosolids Management

We consider the problem of constructing a WWTP to process 10,000 $m^3$ municipal wastewater per day, with average composition given in Table 6.4. The objective is to maximise the NPV and minimise the environmental impacts, while satisfying discharge requirements defined by EU Directive 91/271/EEC on Urban Wastewater Treatment. This includes minimum abatements of 75% total COD, 80% total N and total P, and 90% TSS, equivalent to maximal concentrations of 142.3 mg/L total COD, 7.6 mg/L $NH_4^+$-N, 10.3 mg/L $NO_3^-$-N, 0.82 mg/L $PO_4^{3-}$-P and 25.9 mg/L TSS. The superstructure is shown in Figure 6.4 and consists of 1 source to split wastewater to other treatment/ separation units or sinks, 2 sinks to receive wastewater and sludge after treatment before discharge to the environment or final disposal, 11 treatment/ separation units including conventional wastewater treatment processes, resource recovery units, side stream treatment and sludge treatment units as summarised in Table 6.5 and illustrated in Figure 6.4:

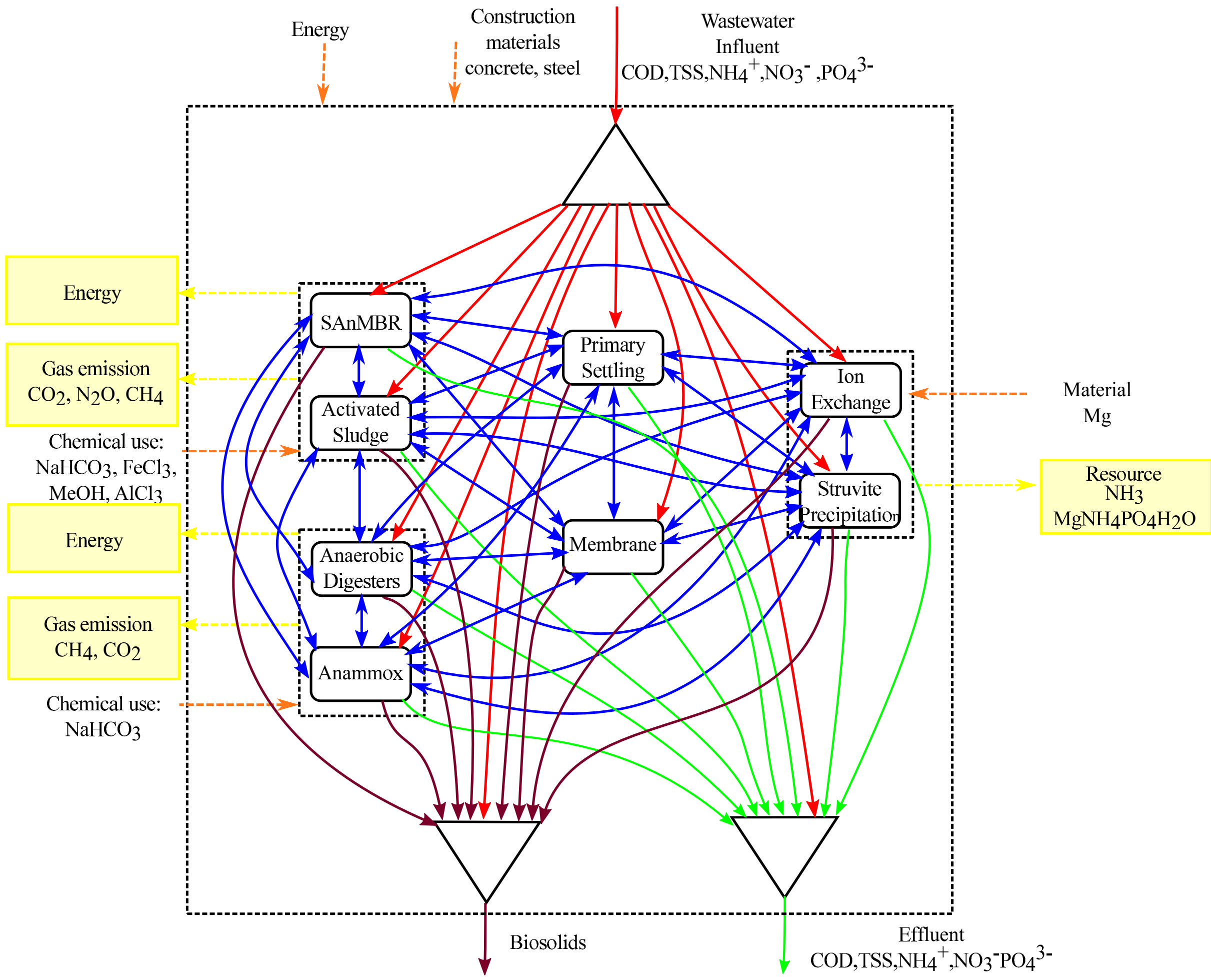



Figure 6.4: System boundaries for the synthesis of a municipal wastewater facility.

Table 6.4: Characteristics of the municipal wastewater.

| Total COD | Soluble COD | TSS | VSS | VFA |
|---|---|---|---|---|
| 569 mg $L^{-1}$ | 129 mg $L^{-1}$ | 259 mg $L^{-1}$ | 231 mg $L^{-1}$ | 10 mg $L^{-1}$ |
| Total N | Ammonia | Total P | Phosphate | Alkalinity |
| 51.6 mg $L^{-1}$ | 38 mg $L^{-1}$ | 7.6 mg $L^{-1}$ | 4.1 mg $L^{-1}$ | 253 mg $CaCO_3$ $L^{-1}$ |

- **Primary Treatment** - the primary clarifier was considered in the superstructure to separate particulate contents from wastewater. It has several impacts on both wastewater and sludge treatment. Results from Chapter 3 and Chapter 4 and other studies have indicated that the primary clarifier can provide benefits in terms of energy recovery, energy reduction and nutrient removal [71].

- **Secondary Treatment** - four different biological treatment units were included in the superstructure: three activated sludge with different configurations and SAnMBR. The first three options are conventional wastewater treatment processes, commonly used and has been proven to be effective for removing organic content and nutrients in both lab and full scales. The SAnMBR is a potential technology in terms of energy-saving and able to improve environmental sustainability [236].

- **Tertiary Treatment** - a membrane filter (microfiltration) was selected in the superstructure with the aim to polish effluent quality in terms of particulate matter before discharge.

- **Sludge Treatment** - anaerobic digestion coupled with dewatering units was used to stabilise and reduce the volume of sludge before disposal using landfills. This technology is commonly used and provides several advantages, especially energy recovery and conditioning of sludge.

- **Side-stream Treatment** - SHARON®/Anammox was selected to be included in the superstructure. It is an innovative and economic approach for ammonium-rich wastewater. Some studies have indicated that this technology can save significant amount of energy and cost because of lower oxygen consumption [237].

- **Recovery Units** - two nutrient recovery units were added in the superstructure to recover nitrogen and phosphorus: ion exchanger and struvite precipitation. As mentioned, we consider SAnMBR as well as anaerobic digestion as the secondary and sludge treatment. Although these technologies are able to perform organic degradation effectively, they have a little effect on nutrient removal. As a result, further technologies may need to remove nutrients to satisfy discharge regulations. Also, both ion exchanger and struvite precipitation can recover nutrients in wastewater and used as fertilisers.

Table 6.5: List of treatment/separation units available in the superstructure.

| Stage | Unit |
|---|---|
| Primary treatment | Primary sedimentation |
| Secondary treatment | Activated sludge with an oxic tank and clarifier |
| | Activated sludge with modified Ludzack-Ettinger |
| | Activated sludge with A2O for phosphorus removal |
| | SAnMBR |
| Tertiary treatment | Membrane filter |
| Sludge treatment | Anaerobic digestion with SRT 15 days |
| | Anaerobic digestion with SRT 20 days |
| Side stream treatment | Anammox |
| Recovery | Ion exchanger |
| | Struvite precipitation |

In this study, design parameters, e.g. SRT, HRT were kept constant for each treatment/separation unit and selected from a given range obtained from engineering guidelines [17]. This is commonly used to design conventional WWTPs, e.g. activated sludge processes. Regarding new technologies where data from engineering guideline is not available such as SAnMBR, the principle design parameters are considered based on information from the literature. For instance, HRT of 12 hrs and SRT of 30 days were chosen based on lab and full scale operating conditions for municipal wastewater available in the literature [238] and these conditions were fed into the process simulator, GPS-X® to simulate performance of the SAnMBR. In this context, the size of each treatment/separation unit can be calculated using the flowrate determined by the optimiser and selected HRT/SRT. Note that in order to limit the number of variables in the surrogate models, multiple instances of the same unit can be considered as part of the superstructure, which correspond to different sets of operating parameters: For example, anaerobic digestion was simulated for two operating SRTs i.e. 15 and 20 days to increase flexibility and this allows decision-makers to identify the optimal design parameters for each technology.

### 6.4.1 Performance of Treatment Units

The performance of the treatment units is approximated based on the simulation outputs using ManTIS3 built in GPS-X® by varing COD, $NH_4^+$-N and $PO_4^{3-}$-P concentrations.

The degradation/removal rates of organic matter, nutrients are regressed using simple surrogate models, either linear or quadratic models of the form:

$$X_{k,c}^{\text{out}} = b_{k,c}^{e} + \sum_{u} m_{k,c}^{e1} X_{k,u}^{\text{in}} + \sum_{u} m_{k,c}^{e2} (X_{k,u}^{\text{in}})^2 \tag{6.7}$$

$$F_{k}^{\text{out}} = F_{k}^{\text{in}} (b_{k,c}^{f} + \sum_{u} m_{k,c}^{f1} X_{k,u}^{\text{in}} + \sum_{u} m_{k,c}^{f2} (X_{k,u}^{\text{in}})^2) \tag{6.8}$$

where $b_{k,c}^{e}$, $m_{k,c}^{e1}$ and $m_{k,c}^{e2}$ are the parameters in surrogate models for the concentration $c$ of unit $k$. $b_{k}^{f}$, $m_{k}^{f1}$ and $m_{k}^{f2}$ are the parameters in surrogate models for the outlet flowrate of unit $k$. Note that the cross term is not included in a general equation above due to the fact that accuracy of the predictions is seldom improved compared to the simplified equation. The performance models as examples are shown in Figure 6.5 for an anaerobic digester unit. For some treatment units producing sludge, the flowrate and concentrations of sludge can be predicted based on the surrogate models as follows:

$$X_{k,c}^{\text{was}} = b_{k,c}^{we} + \sum_{u} m_{k,c}^{we1} X_{k,u}^{\text{in}} + \sum_{u} m_{k,c}^{we2} (X_{k,u}^{\text{in}})^2 \tag{6.9}$$

$$F_{k}^{\text{was}} = F_{k}^{\text{in}} (b_{k,c}^{wf} + \sum_{u} m_{k,c}^{wf1} X_{k,u}^{\text{in}} + \sum_{u} m_{k,c}^{wf2} (X_{k,u}^{\text{in}})^2) \tag{6.10}$$

where $b_{k,c}^{we}$, $m_{k,c}^{we1}$ and $m_{k,c}^{we2}$ are the parameters in surrogate models for the sludge concentration $c$ of the unit $k$. $b_{k}^{wf}$, $m_{k}^{wf1}$ and $m_{k}^{wf2}$ are the parameters in surrogate models for the sludge flowrate of the unit $k$.

Regarding the membrane filters (ultrafiltration) and primary clarifier, the performance was simulated based on a split fraction of the solid components, which can affect total suspended solids and the particulate fraction of COD. In the simulation of these two units, it was assumed that no biological reactions occurred, and treatments had no effect on soluble components. Due to the unavailability of ion exchanger data in GPS-X®, the performance of this unit was modelled based on a Langmuir adsorption isotherm combined with the experimental data derived from a study by Malekian et al. [239]. It was assumed that the adsorbent only absorbed ammonium, but had no effect on other components, while the concentration of the suspended solids entering the ion exchange unit was assumed to be less than 12 mg/L to prevent adsorbent pore clogging.

The capital and operational costs of all the units were estimated using CapdetWorks®, and fitted with a linear regression model as a function of the input flowrate within the operational range for a given volume. In addition to treatment/separation units, a combined heat and power (CHP) unit was modelled in this study for electrical and thermal power generation from biogas (CHP is not included in Figure 6.4 for simplicity but it would be taken into account when the anaerobic digestion process is selected) . The CAPEX and OPEX of CHP in the model were based on the data published by the Department of Energy & Climate Change [240].

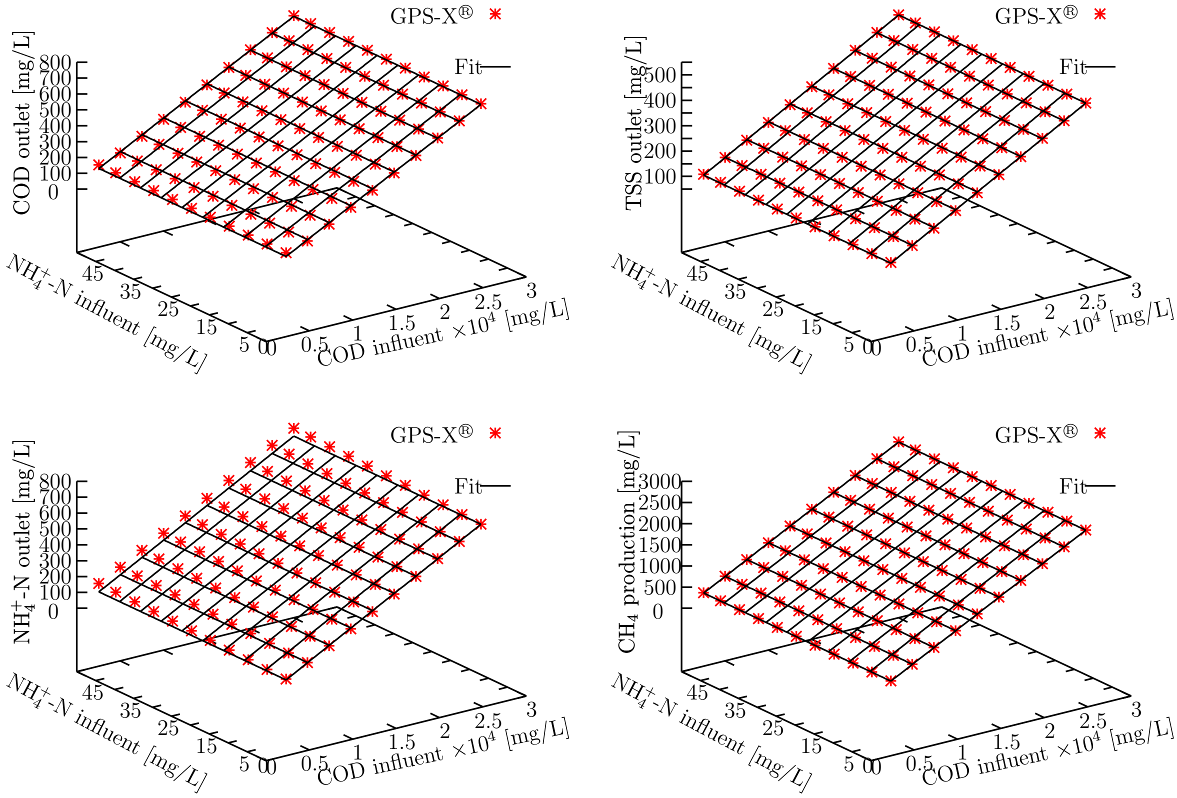



Figure 6.5: Subset of regression models for performance of an anaerobic digester unit. Top left: COD effluent; Top-right: TSS effluent Bottom-left: $NH_4^+$-N ; Bottom-right: $CH_4$ production as a function of COD and $NH_4^+$-N influent.

### 6.4.2 Single-objective Optimisation

The optimal configuration for NPV maximisation is shown in Figure 6.6. Approximately 91% of the wastewater stream is processed in the activated sludge unit with enhanced phosphorus removal efficiency (A2O) and clarifier (not shown in Figure 6.6), before being mixed with the remaining stream and discharged into receiving waters. The sludge derived from activated sludge unit is processed in the anaerobic digestion unit with an SRT of 20 days, and the supernatant generated is fed back to the activated sludge unit; the remaining sludge residue is disposed of to landfill. The minimum reduction requirement for TSS (90%) is the most restrictive, while the effluent satisfies all other discharge requirements. The NPV for this optimal configuration over a period of 20 years is estimated as - £7.69 million, with the breakdown costing analysis including CAPEX, OPEX and SALES shown in Table 6.7. CAPEX is the dominant factor in deriving the NPV, and thus only a small number of treatment units (to meet the discharge constraint) are selected to achieve NPV maximisation in this optimisation solution. A long rather than short SRT is suggested as the optimal configuration for the anaerobic digestion unit, which can be explained by the greater amount of biogas produced under longer SRTs. However, the optimal configuration for the economic objective causes high environmental burdens on GWP100 due to the energy-intensive activated sludge unit, as well as its high GHG emission profiles (e.g. $N_2O$ evolved from biological treatment). In addition, this configuration produces environmental burdens on eutrophication which are mainly caused by the remaining COD, $NO_3^-$-N, $NH_4^+$-N and $PO_4^{3-}$-P in the effluent and sludge residues. Note that bypassing the wastewater stream directly to the water receiving body may not practically reasonable. The optimiser selects this configuration as the maximisation of NPV because sending more amount of wastewater can increase the size of treatment units and this could potentially lower the NPV. It is also possible to set the constraints that do not allow the wastewater stream to be sent directly to the sink. It is found that the optimal configuration is similar to Figure 6.6 with no wastewater stream bypassing to the sink directly. However, the NPV would be lower (worsen) around 9% due to the larger size of the activated sludge and anaerobic digestion units.

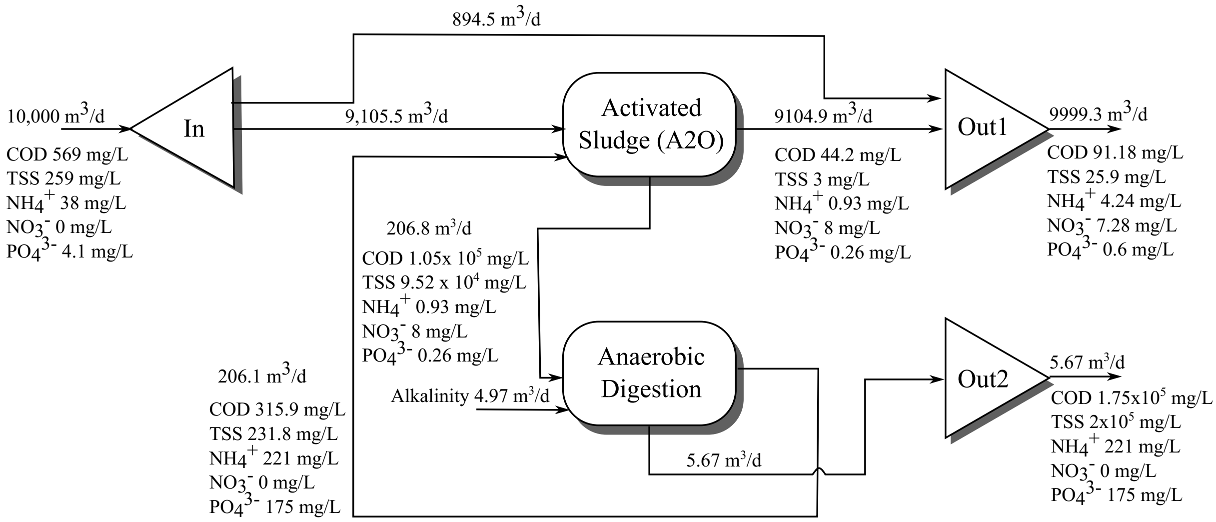



Figure 6.6: Illustration of the optimal result (maximisation of NPV)

Another important step in the WWTP decision-making tool development is model verification to demonstrate the model consistency, completeness and correctness. The objective of model verification is to check the quality of the model outputs, and identify further modifications to ensure that the solution can address the problem. As stated in section 5.2.1, surrogate models require verification by comparing the optimisation results with outputs from the process simulator, and the progressive update of the simulated data to improve model outcomes. Thus in this study, model verification was carried out through error analysis by comparing the superstructure-based optimisation results with full-scale wastewater simulation outputs. Figure 6.7 demonstrates an example of model verification, i.e. the NPV-maximisation optimal result verified and implemented in the wastewater treatment simulator. The results from superstructure-based optimisation, and the full-scale wastewater treatment simulation are summarised in Table 6.6, where the average deviations of both model results are lower than 5%. Generally, deviations or the differences between the superstructure-based optimisation and the full-scale wastewater treatment simulation (verification) decrease gradually with the number of iterations of the surrogate model updating, because wastewater treatment process simulation results are influenced by multiple factors, e.g. wastewater compositions and recycle streams. The surrogate model is updated iteratively and this would affect accuracy of the model predictions. In this case, the optimal configuration was not affected by the iteration process because the surrogate models generated for describing treatment/separation unit performance did not change significantly throughout the iteration process. It is interesting to note that it is possible to obtain results with different configurations for each iteration though because the optimisation model is based on the surrogate model or the simplified approximate model. As the surrogate model is updated iteratively, it would be possible that the updated surrogate model is changed from the previous iteration.

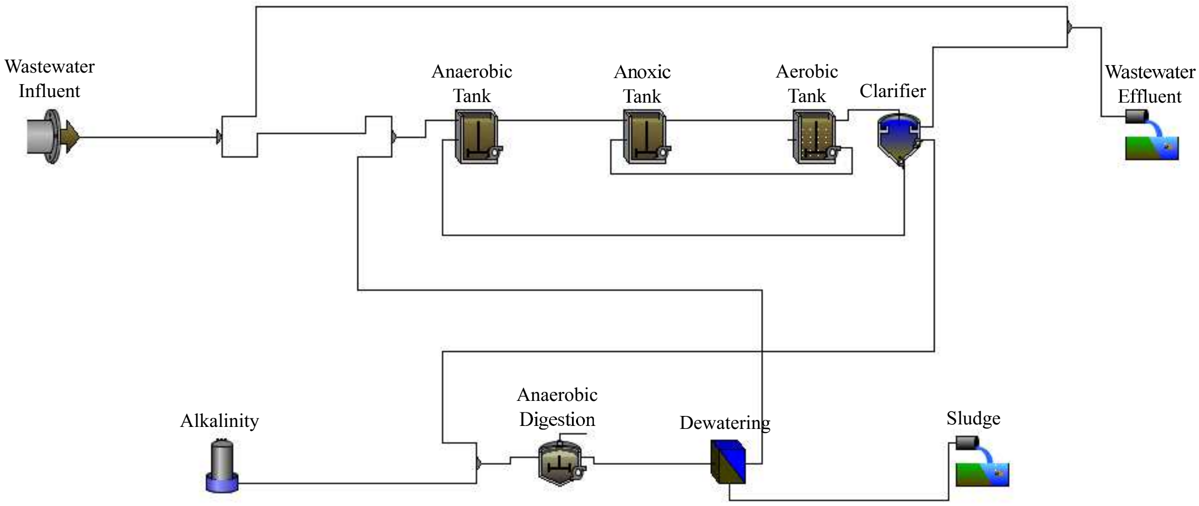



Figure 6.7: Illustration of full-scale wastewater treatment simulation in GPS-X®.

Table 6.6: Comparision of the optimisation result obtained from GAMS with the full scale WWTP simulation in GPS-X®.

| Stream | Component | Unit | Optimisation GAMS | Simulation GPS-X® | Deviation [%] |
|---|---|---|---|---|---|
| Effluent | Flow | $m^3/d$ | 9999 | 9996 | 0.03 |
| | COD | mg/L | 91.18 | 91.08 | 0.11 |
| | $NH_4^+$-N | mg/L | 4.24 | 4.26 | 0.47 |
| | $NO_3^-$-N | mg/L | 7.28 | 7.45 | 2.28 |
| | $PO_4^{3-}$-P | mg/L | 0.60 | 0.59 | 1.69 |
| | TSS | mg/L | 25.9 | 25.76 | 0.54 |
| Sludge | Flow | $m^3/d$ | 5.67 | 5.96 | 4.86 |
| | COD | mg/L | $1.75\times10^5$ | $1.83\times10^5$ | 1.33 |
| | $NH_4^+$-N | mg/L | 221 | 218.1 | 6.51 |
| | $NO_3^-$-N | mg/L | 0 | 0 | 0 |
| | $PO_4^{3-}$-P | mg/L | 175 | 164.3 | 6.51 |
| | TSS | mg/L | $2\times10^5$ | $2\times10^5$ | 0 |
| Gas | $CH_4$ | $m^3$/day | 342 | 369.93 | 7.55 |
| | $CO_2$ | $m^3$/day | 250 | 268.71 | 6.96 |

The two environmental impacts GWP100 and eutrophication were also investigated using single-objective optimisation. Both case studies show similar process configurations (Figures 6.8 and 6.9). The optimal configuration for minimising GWP100 shows that around 52% of the wastewater stream is sent to the SAnMBR, and then mixed with the remaining 48% (bypass directly), and the mixed stream is sent to the membrane filter for particulate fraction separation. Sludge produced in the SAnMBR is processed in the anaerobic digestion units (SRT 20 days), where the supernatant produced is fed back to the SAnMBR and the digestate cake produced is collected for disposal. The supernatant from the membrane filter is sent to the recovery units which consist of an ion exchanger and struvite precipitation for recovering nitrogen and phosphorus, respectively; the treated supernatant is then discharged to the environment. Sludge from the membrane filter is recycled back to the SAnMBR. A similar configuration for the minimisation of eutrophication impacts was also found (Figure 6.9). 100% of the wastewater stream is treated by a SAnMBR and partially processed in the membrane filter before mixed with the remaining fraction and sent to the nutrient recovery units (e.g. ion exchanger and struvite precipitation). Partial sludge from the membrane filter is recycled back to the SAnMBR and anaerobic digestion. The selection of a SAnMBR rather than activated sludge in the environmental optimisation runs can be explained by the superior environmental profiles of the SAnMBR compared to activated sludge units on GWP100 and eutrophication. Moreover, the nitrogen and phosphorus nutrient recovery bring environmental credits by fertiliser substitution, which is another driver of the optimisation outcome. The optimisation model shows that a reduction in the GWP100 and eutrophication burdens can lead to a lower NPV, whereas the addition of a membrane filter can potentially reduce the environmental impacts, but incurs higher installation and operational costs.

### 6.4.3 Multi-objective optimisation

This final section focuses on multi-objective optimisation to generate the Pareto frontiers to provide insight into the trade-offs between conflicting objectives in this study. Overall,

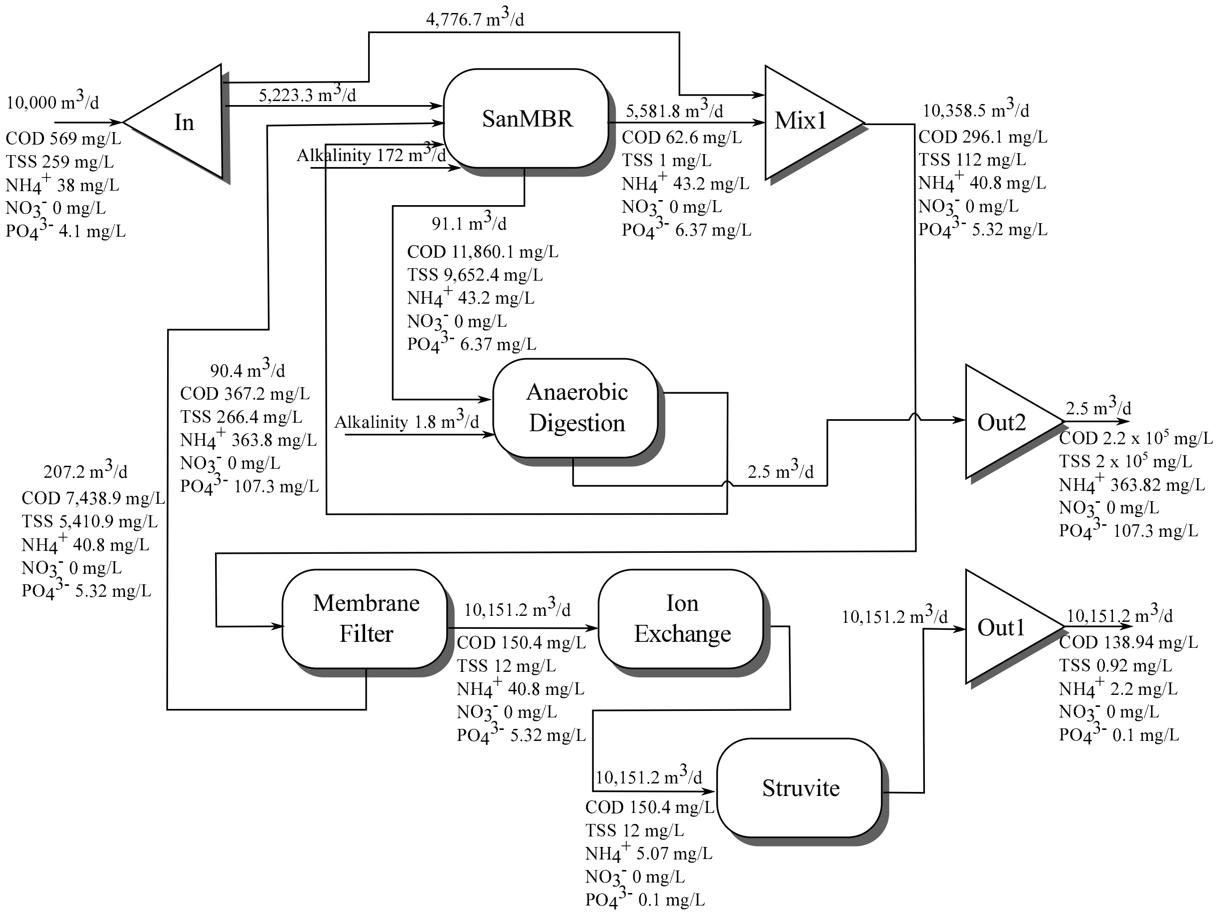



Figure 6.8: Illustration of the optimal result (minimisation of GWP100).

three objective functions; NPV, GWP100 and eutrophication were optimised, and the derived Pareto optimal solutions are shown in Figure 6.10. The Pareto frontier for trade-off between conflicting NPV, GWP100, and eutrophication can be identified. Note that each Pareto optimal solution corresponds to a unique process configuration with specific operating conditions and effluent quality from all Pareto optimal solutions can satisfy discharge regulations. In this case, all of the NPV values are negative so it would be better

Table 6.7: Cost and environmental analysis for the case study.

| Flowsheet | max NPV | min Eutrophication | min GWP100 |
|---|---|---|---|
| CAPEX, M£ | -5.42 | -11.04 | -8.72 |
| OPEX, M£/year | -0.45 | -0.77 | -0.61 |
| SALES, M£/year | 0.24 | 0.45 | 0.37 |
| NPV, M£ | -7.69 | -14.41 | -11.22 |
| GWP100, $\times 10^4$ $kgCO_2e$ | 23.2 | 1.91 | 0.66 |
| Eutrophication, $\times 10^2$ $kgPO_4^{3-}e$ | 4.96 | 1.55 | 2.88 |

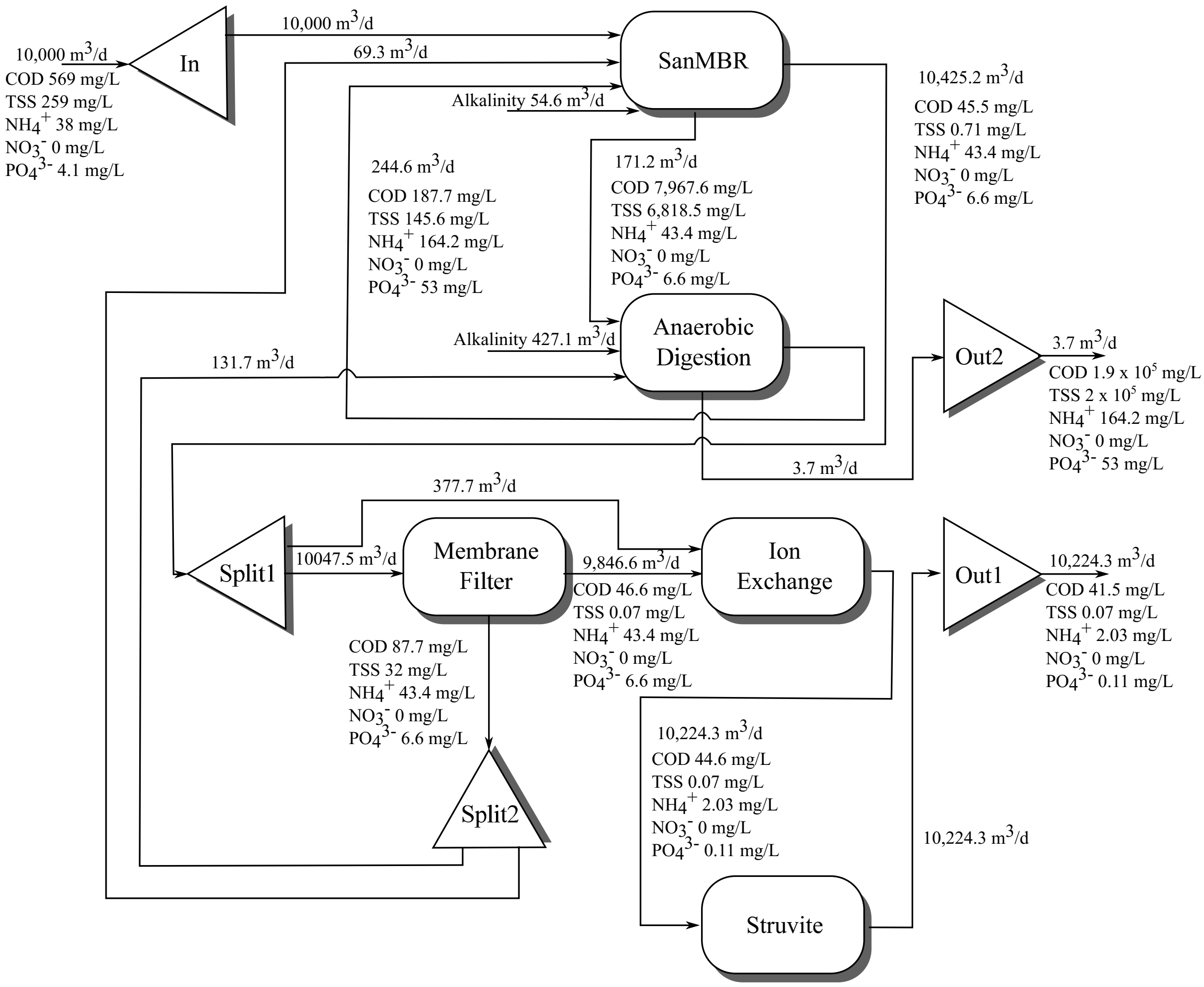



Figure 6.9: Illustration of the optimal result (minimisation of eutrophication).

to clarify that the higher NPV (or lower negative ) mean that the project is better in terms of economic consideration. The optimal solutions on the bottom of Figure 6.10 emphasize more on minimise the environmental impacts i.e. GWP100 and eutrophication, while the optimal solutions on the top of Figure 6.10 yield maximising the NPV. Expectedly, there is a trade-off among three objectives and the NPV is sensitive to both eutrophication and GWP100. A small change in either eutrophication or GWP100 can lower the NPV significantly. Decision makers can choose the optimal design on the Pareto frontier based on the preference. In this case study, a number of discontinuous planes arising from the optimal configurations were changed to satisfy the constraints. This situation is commonly found in the chemical engineering design [213]. When environmental constraints are tightened, the optimiser selects different process configurations in terms of selected units and interconnections corresponding to the stricter constraints. Further inspection reveals that there are three clear lines of Pareto optimal solutions: A and B corresponding to the resource recovery facilities with (Figure 6.8 and 6.9) and without membrane filters; C corresponding to the conventional wastewater treatment facility (Figure 6.6). More detail about the optimal process configurations is available in appendix 11. Changing the optimal solutions from C to B would lower the NPV around 40% but the environmental impacts i.e. GWP100 decreases significantly from $23{\times}10^4$ to $1.7{\times}10^4$ $tCO_2$ (13 folds). This may be particularly useful in the near future when the carbon tax rate is higher. To better interpret the trade-offs among the three objectives, the Pareto frontiers achieved for two objective functions are discussed as follows:

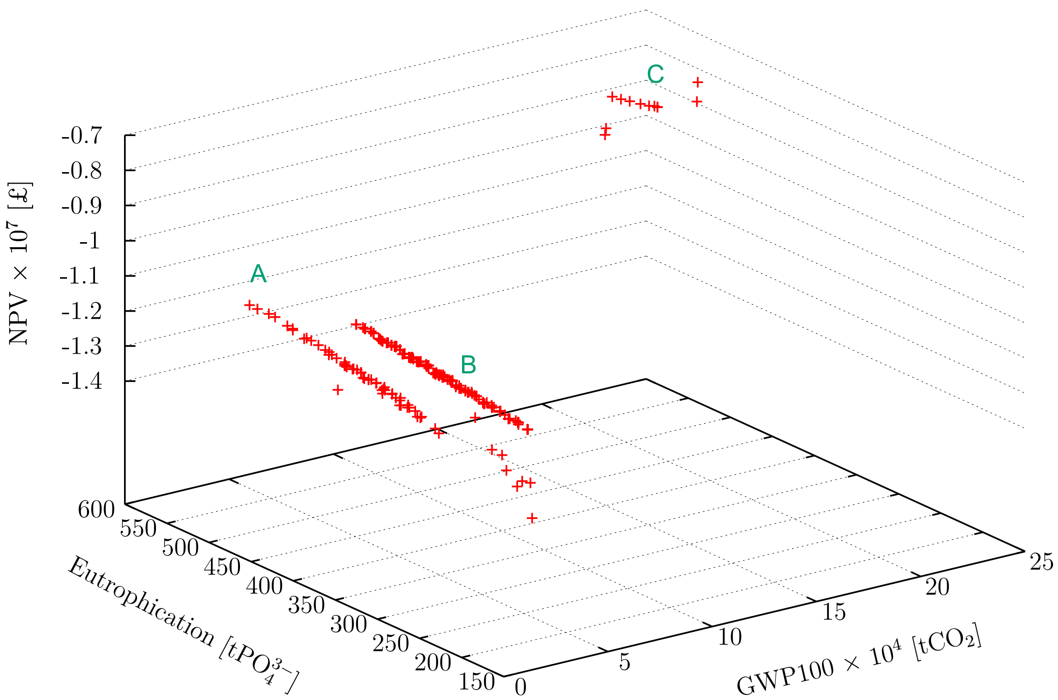



Figure 6.10: Pareto frontier of three objective functions.

### 6.4.3.1 NPV and GWP100

The NPV and GWP100 objectives were optimised simultaneously using the multi-objective programming $\varepsilon$-constraint method, where GWP100 was treated as a constraint. Figure

6.11 demonstrates a set of Pareto solutions where the conflicting objectives between NPV and GWP100 are found and each point on the Pareto front represents a unique model parameterisation. Along the Pareto frontier, a decrease in GWP100 is accompanied by a reduction in the NPV. The maximised NPV solution has the highest impact on the environment in terms of GWP100, whereas the most environmentally friendly solution can be achieved at the expense of a minimised NPV. This is because the minimisation of GWP100 as a resource recovery facility in Figure 6.8 requires the larger number of treatment units to satisfy the conditions and large amount of CAPEX. Although more resources can be recovered, this cannot be compensated by the higher CAPEX. As a result, the NPV would be lower (minimised NPV). Each solution represents a WWTP configuration under a set of specific conditions, and hence the solutions on the frontier show how the model seeks for alternative solutions with varying environmental targets. To satisfy the imposed environmental requirements, the plant configurations and operating conditions were adjusted for each case in the model. For example, the conventional WWTP (A2O) with a energy recovery unit (anaerobic digestion) can yield higher NPV but it delivers negative impacts on GWP100 due to high energy consumption and induced direct GHG emissions. The resouce recovery facility is likely to be economic unfavorable due to high investment, but can potentially produce beneficial impacts due to the credits obtained from nutrient recovery. In addition, a discontinuous Pareto frontier is observed in Figure 6.11, which is caused by changing the process configuration or adding treatment/separation unit. More specifically, the discontinuities may result from the fact that there is no optimal solution found at the certain ranges of $\epsilon$-constaint or the better solution with the new optimal configuration is found at the lower $\epsilon$-constaint. For instance, changing from the conventional wastewater treatment plant (Figure 6.6) to the resource recovery facility (Figure 6.8 and 6.9) could significantly reduces the GHG footprint, but incurs high installation and operational costs as mentioned above.

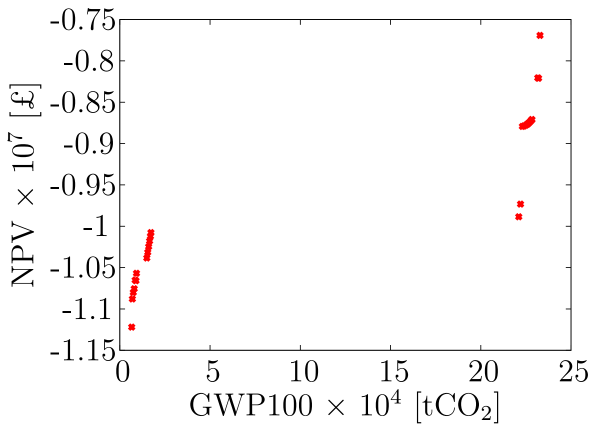



Figure 6.11: Pareto frontier between GWP100 and NPV

#### 6.4.3.2 NPV and eutrophication

The Pareto frontier for trade-off between conflicting NPV and eutrophication objectives is shown in Figure 6.12. The identified set of optimal solutions consists of different plant configurations and specific conditions from conventional wastewater treatment plants (A2O) to the resource recovery plants. Decreasing overall eutrophication impacts leads to an increase in NPV; the optimiser selects a conventional activated sludge process with anaerobic digestion as the NPV optimal solution, as shown in Figure 6.6. Note that the main source of eutrophication is from effluent and sludge production. The improved eutrophication performance from (ca. 500 to 350 $tPO_4^{3-}$-P) is achieved by decreasing the bypass stream, and sending it to the treatment units to minimise contaminants discharged into the receiving waters. Changing the eutrophication profile in this range would slightly lower the NPV around 14%. Although more resource can be recovered, it cannot be compensated by the higher CAPEX and OPEX from the larger size of unit operations and higher operating cost. With further enhancement of the eutrophication profile (ca. 350 to 155 $tPO_4^{3-}$-P), the configuration shifted from wastewater treatment to the resource recovery facility, and hence lower contaminants in the discharged effluent, and a higher credit from N&P nutrient recovery could be achieved. It is infeasible to obtain the optimal solution when the eutrophication is lower than 155 $tPO_4^{3-}$-P.

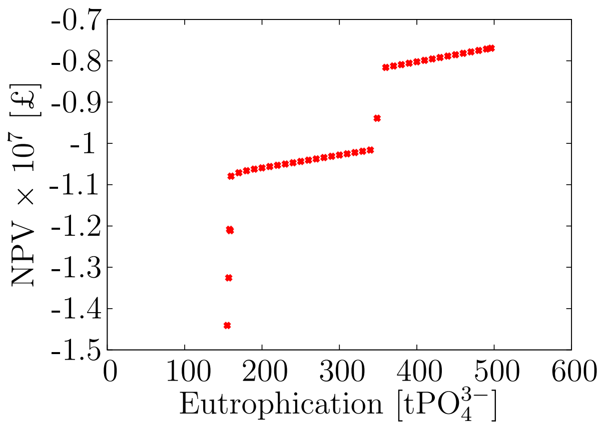



Figure 6.12: Pareto frontier between eutrophication and NPV

#### 6.4.3.3 GWP100 and eutrophication

The Pareto frontier for conflicting environmental issues, i.e. eutrophication vs. GWP100, was obtained by treating eutrophication as a constraint, and solving the resulting single-objective problem. All optimal configurations presented in Figure 6.13 along the Pareto frontier are based on the selection of a SAnMBR as the biological treatment, followed by N&P resouce recovery units, including ion exchange and struvite precipitation. The results show that GWP100 is highly sensitive to eutrophication. A slightly lower eutrophication profile (from ca. 300 to 150 $tPO_4^{3-}$) can lead to a significantly higher GWP100 from $0.6\times10^4$ to $2\times10^4$ $tCO_2$. Further inspection reveals that the most environmentally friendly solution can potentially be achieved by introducing nutrient recovery on the effluent from existing WWTP facilities. The eutrophication impacts can be decreased by reducing the bypass stream, sending to the SAnMBR unit, and increasing the nutrient recovery rate, which not only leads to a reduction in the eutrophication precursors (e.g. $NO_3^-$-N $NH_4^+$-N and $PO_4^{3-}$-P) in the effluent, but also brings environmental benefits due to fertiliser substitution. To achieve optimised GWP100 profiles, the optimiser tends to choose an increasing bypass stream which in turn lowers the flowrate to the treatment/separation unit, - the resulting reduced unit size and energy consumption could benefit GWP100 profiles.

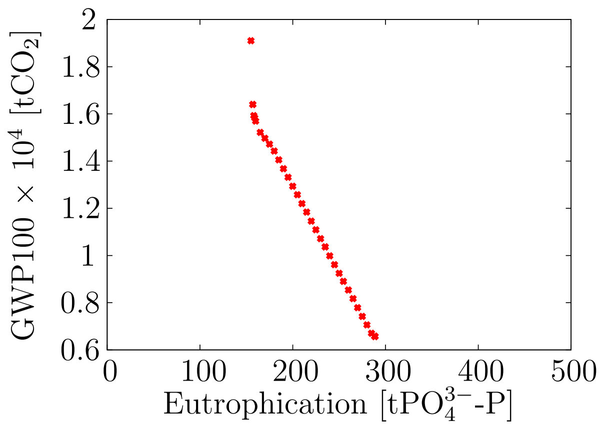



Figure 6.13: Pareto frontier between eutrophication and GWP100

## 6.5 Summary

This chapter has presented an extended WWTP synthesis modeling framework based on enviroeconomic optimisation. The extended model is configured to integrate wastewater and sludge treatment into a single WWTP system, and incoporates LCA into a multi-objective optimisation framework to achieve a sustainable WWTP design. With current computational capabilities, however, it would be computationally intractable to solve a complex WWTP system with multiple scales, and great uncertainties, e.g. identification of promising wastewater treatment facilities from hundreds or thousands of alternatives using global optimisation techniques. The proposed methodology allows us to solve such complex optimisation problems by developing simple surrogate models for unit performance and costing data based on state-of-the-art wastewater treatment simulators. Typically, surrogate models provide a rough approximation for the actual performance of complex systems, and contain significant uncertainty. To solve this issue, we proposed a model verification approach to refine these surrogate models iteratively. The applicability of extending the modeling framework has been illustrated through a case study in municipal wastewater treatment with biosolids management. The set of Pareto optimal solutions determined optimisation suggests that significant environmental improvements in GWP100 and eutrophication can be achieved through a modification of the process configuration, or operating conditions. Decision-makers can use this approach as a decision-making tool to choose the most approapriate wastewater treatment facilities based on their preference.

Also, it is possible to analyse more detail in terms of economic and environmental aspects to obtain a better understanding for each optimal Pareto solution to identify the trade-off solutions. Overall, the results show that accounting for LCA considerations early on in the synthesis problem may lead to dramatic changes in the optimal process configuration, thereby supporting LCA integration into decision-making tools for wastewater treatment alongside economical selection criteria.

# Chapter 7

# Discussions

The results shown in the previous chapters lead to several discussions. This thesis presents the importance of the model-based methodology as a decision-making tool used to identify the key improvement opportunities for existing WWTP operation and to design new wastewater treatment/resource recovery facilities to achieve sustainability defined as maximisation of economic objectives and minimisation of overall environmental impact including GHG emissions. Regarding existing WWTP operation, plant-wide models can generally be used as a decision-making tool for engineers, plant managers and environmental regulators to evaluate the performance of a plant-wide system in setting the targets and limits of the WWTP. Also, it can be used to optimise operational strategies and plant performance if the WWTP is upgraded or retrofitted. For design of new wastewater treatment facilities, the optimal layouts of future wastewater treatment facilities for the energy and nutrient recovery using cutting-edge treatment technologies can be developed through the application of the model-based methodology. Using the powerful capability of the modeling and optimisation techniques, the best possible plant layout among hundreds or thousands of process alternatives can be systematically selected for tomorrow's wastewater treatment facilities. More detail of the key findings and limitations of this thesis is as follows.

## 7.1 Applications in WWTP Operation

Improving existing WWTP operation with regards to energy use, effluent quality and GHG emissions can be identified through the model-based methodology. A key finding in this study shows the importance of plant-wide evalution using the model-based methodology and the inherent advantage of incorporating GHG emissions along with effluent quality. The plant-wide models developed can be used to identify what level of nutrient discharge, energy consumption and GHG emissions should be reduced and what impact further reduction in nutrient discharges has on the overall plant's performance, e.g. a significant increase in energy consumption as well as GHG emissions. This information will be used to identify the main trade-off between nutrient discharge, energy consumption and GHG emissions without compromising each other. For example, a decrease in the DO set-point from 2 mg/L to 1 mg/L can lead to a reduction in the aeration energy (15%) and total nitrogen 1 mg/L while ammonia discharge is kept at a minimum and an increase of around 2% in the overall GHG emissions (A decrease in the aeration energy is counter-balanced by an increase of $N_2O$ emissions). These overall GHG emissions were compared to a similar study and the results also show similar trends as well as in a medium range of several studies regarding the GHG emissions [171, 172]. Although the lower DO set-point provides a benefit in terms of energy consumption, the overall GHG emissions could be largely due to the higher $N_2O$ emissions at the lower DO set-point. This is a clear advantage of incorporating GHG emissions as a criterion along with effluent quality. Other scenarios were also investigated including influent spliter, MLR and SRT to examine the potential reduction of nutrient discharge, energy consumption and GHG emissions. Similar to the DO-setpoint case, manipulating SRT can potentially reduce the aeration and nutrient discharges but this can lead to an increase in $N_2O$ emissions due to incomplete nitrification. Regarding MLR and influent spliter, it is important to point out that the nitrate concentration can be reduced down to approximately 3 mg/L. This reduction leads to an increase in $N_2O$ emissions due to carbon availability limits capability of denitrification affecting nutrient discharge and the GHG emissions in terms of $N_2O$

emissions. Adding the external carbon would potentially enhance nutrient removal and reduce GHG emissions. The potential of reverse osmosis (RO) was also investigated. The reverse osmosis was installed at the WWTP and only a partial amount of water from the final effluent is sent to the RO to increase the recycled water. The model predictions are able to identify an increase of energy consumption when the full amount of water from the final effluent is sent to the RO. Expectedly, the nutrient concentration was reduced significantly and provided a quality of water which was similar to potable. However, this was compensated by a significant increase in energy consumption and GHG emissions.

Another interesting study regarding the improvemence of existing WWTPs was to investigate the feasibility of systematic optimisation. Similar to the previous study, this study shows the importance of the plant-wide evaluation using the model-based methodology to a full-scale WWTP (owned and operated by Sydney Water). However, the key finding was that it shows the potential capability of using the systematic optimisation as a decision-making tool to identify an inherent trade-off between effluent quality and nutrient discharges and investigate the optimal operational strategies. Also, it is possible to enhance robustness of the operational strategies to maintain optimal performance even though the conditions are different from nominal conditions. This study has highlighted that nutrient discharges in terms of $NH_4^+$-N and $NO_3^-$-N can be reduced significantly without compromising energy consumption or it is possible to reduce these significantly while keeping the level of nutrient discharges the same. The current operation of the WWTP in the study is based on the high standard set-point to maintain suitable effluent quality to prevent unpredictable situations, e.g. heavy rainfall. As a result, the treated effluent is usually much better than the requirements enforced by the environmental regulators and it leads to significantly higher energy consumption. This shows the excellent potential for systematic optimisation to improve a WWTP with a large number of process interactions between liquid and sludge treatment stages, as well as other conflicting objectives are found. Typically, the model-based methodology relys on simulation but the problem is that the optimal solution cannot be guaranteed through the model simulation and it is time-consuming to investigate several key operating variables on operational strategies of the WWTP. With capabilities of the model-based methodology and optimisation techniques, several key operating variables can be adjusted to obtain the optimal operational strategies. Although the results of the model-based methodology is specific for this case study, the proposed approach can be generic and applied to other wastewater treatment systems to develop their optimal operational strategies or identify the main trade-off between conflicting objectives, e.g. effluent quality and energy consumption typically found in wastewater treatment processes.

It is important to point out that although the plant-wide evaluation in this study can provide promising results, there are some limitations regarding the plant-wide models. The operational data is currently recorded online and offline in a database system. However, it is found that large sets of data are not frequently recorded and some are incorrectly recorded (outliers). This would affect the accuracy of model predictions. With limited availability of operational data, several assumptions needed to be made throughout the study. More data availability including consistent data collection and analysis would reduce the uncertainty arising from model assumptions and make the model predictions more realistic. For example, calibrating the biological treatment is aimed to capture the average trends and the daily variation of the WWTP, in order to predict the dynamic behaviour. Operational data should be consistently collected/measured or collected from experimental design, e.g. the tracer test or the determination of kinetic and stoichiometric parameter (which is required for the model-based methodology to improve quality of model calibration). Also, the energy consumption of pumps was calculated based on the assumption of constant efficiency due to limited data availability of pump calculation. Although this approach can provide a first approximation, it would be better to improve the predictive capability by consistently collecting data.

## 7.2 Applications in Design of Wastewater Treatment Facilities

In this study, a superstructure-based optimisation is developed and its applicability is highlighted through case studies to design new wastewater treatment/resource recovery facilities to achieve economic and environmental sustainability. The key finding is that the proposed methodology using superstructure optimisation together with surrogate models can be used as a decision-making tool to design a globally optimal wastewater treatment facility. It is computationally intractable to design the globally optimal wastewater treatment facility with regards to the current computational capability and optimisation techniques due to high complexity of wastewater treatment processes and a large number of process alteratives. The surrogate model is an approximate model that is simple but reliable enough to represent the wastewater treatment process. An inherent advantage of using the surrogate model is that it can provide the approximated performance of treatment units, allowing the use of global optimisation techniques to search for the global optimality. The global optimisation techniques used are important because there is a presence of bilinearities from the mass balance and this can result in multiple local optimal solutions. As such the surrogate model is more accurate in representing the performance of treatment units compared to constant values which are typically used in several applications of the superstructure-based optimisation [21, 22]. The surrogate model can be developed based on the simulation results or data from experiments to describe the behaviour for which is not available. It is important to point out that the case study presented in Chapter 5 is relatively simple because it was used to proof the concept of this approach that it is computationally tractable to design the complex wastewater treatment facilities. The optimal solutions show promising resource recovery facilities to recover resources from industrial wastewater. However, the CAPEX is significantly higher and it cannot be compensated by the small profit from recovering resources so the NPV is negative. More detail or the complex case study was presented in Chapter 6. The sludge management and LCA to evaluate the environmental impacts were incorporated into the unified optimisation framework to provide the complete picture of sustainability. However, this requires the use of multi-objective optimisation to deal with conflicting objectives and identify trade-offs. Design of a municipal wastewater facility with a potential to recover resources was presented as the case study. The set of optimal solutions corresponding to different process configurations and specific operating conditions were presented on the Pareto front. The decision-makers can select the optimal solution or process configuration based on their preference on the Pareto front. It is found the conventional WWTPs can provide the advantage in terms of the economic aspect but are not good for the overall environmental impacts because of high energy consumption and GHG emissions. The resource recovery facilities, on the other hand, provide less environmental impacts but are not good in terms of the economic aspect because a large number of recovery units are required. Similarly, the case studies presented are quite specific, but the proposed approach can be generic and applied to design other wastewater treatment facilities. Although the proposed approach is a powerful tool used to design the promising wastewater treatment facilities, a limitation of the proposed approach is that the surrogate model or the approximate model needs to be updated iteratively to improve accuracy and completeness because wastewater treatment processes are complex and consist of several variables to describe their behaviours. The surrogate model usually provides a rough approximation of the actual process so it may carry significant uncertainty and one way to reduce uncertainty or improve accuracy is to update the surrogate model iteratively to refine the model.

# Chapter 8

# Conclusions and Future Directions

## 8.1 Conclusions

The main objective of this thesis was to develop decision-making tools for WWTP design and operation. Wastewater treatment facilities are used to ensure a degree of purification to comply with discharge regulations, whilst keeping cost and environmental impacts to a minimum. With powerful capabilities of mathematical modeling, we proposed to use a model-based methodology as a decision-making tool to improve operational strategies of existing WWTPs and design new wastewater treatment/resource recovery facilities. The main contributions and novelty are as follows.

### 8.1.1 Improved Operation of Existing WWTPs

The first contribution of the thesis was to apply the model-based methodology to provide a better understanding of the trade-off between effluent quality, energy use and fugitive emissions. The methodology relies on a scenario-based simulation and optimisation approach and has been applied to two conventional activated sludge plants owned and operated by Sydney Water. An inherent advantage of the methodology is that it can be used for analyzing other "what-if" scenarios as well as for assessing the performance of other WWTPs – provided that mathematical models can be developed/calibrated for those plants. The key novelty in this study is that the developed models can provide a better understanding of what levels of nutrient discharges, energy consumption as well as GHG emissions can be reduced and what impact further reduction in nutrient discharges has on the overall plant performance, e.g. a significant increase in energy consumption and GHG emissions. This type of information is necessary in order to negotiate targets and limits of the WWTP in the near future. Also, the model-based methodology with systematic optimisation allows the modelers to obtain the optimal operational strategies and to incorporate uncertainty into the framework to robustify the operational strategies. More specifically, the main outcomes and insights obtained through the thesis are summarized as follows:

For the first plant (a simulation-based approach), the model-based methodology is used to evaluated the plant-wide performance. It has been found that GHG emissions as a criterian along with effluent quality and energy consumption can provide a better of the trade-off between effluent quality, nutrient discharge and GHG emissions. Adjusting the key operating variables, e.g. DO set-points, MLR and influent splitter is able to improve the performance in one aspect, e.g. energy consumption but it may worsen the other aspects, e.g. GHG emissions. Such trade-offs can be identified by the capabilities of the model predictions. A large reduction of the aeration needs (up to 10-20%), and thus in energy consumption, appears possible by reducing the DO set-point down to a certain value. The DO set-point is found to be particularly sensitive though, and too low a set-point might increase the concentration of $NH_4^+$ in the effluent as well as the $N_2O$ emissions dramatically. The simulation results also suggest that decreasing the SRT could be beneficial in terms of reducing the TN effluent level (up to 1 mg/L), yet this might be accompanied by an increase in $N_2O$ emissions. In addition, reductions in the concentration of $NO_3^-$ in the effluent could be achieved, at the cost of a small energy penalty, by increasing the MLR flowrate or increasing the wastewater split between stages 1/2 and 3 as long as large enough quantities of carbon substrate are available for denitrification. The lack of carbon substrate might however result in partial denitrification, and hence larger $N_2O$ emissions. To remedy this situation, increasing the available carbon substrate for denitrification appears possible. Another possibility would be adding an external carbon source. While reverse osmosis allows a much higher treatment level than the current effluent standards (TN down to 0.3 mg/L), it also inevitably entails a high energy penalty and thus GHG emissions (up to 50%). In making the connection with the modelling work, it might only prove necessary to send a fraction of the treated effluent for polishing in reverse osmosis; the rest of the treated effluent would be directly discharged in the river system, thereby reducing the energy consumption.

For the second plant (an optimisation-based approach), the systematic optimisation is able to simultaneously adjust the key operating variables to optimise the WWTP. The main trade-off between energy consumption and nutrient discharges can be optimally identified. Consequently the optimal operational strategies can be developed to reduce energy consumption without compromising effluent quality. Also, it is able to incorporate uncertainties into the framework to develop the optimal operational strategies with enhanced robustness. The developed tool can expectedly be applied to other systems to identify the key trade-off between conflicting objectives and enhance robustness of operational strategies. More specifically, reduction in energy consumption (20-25%) is possible via operational changes (DO set-point in the aeration tank, RAS, WAS and MLR flowrates). Nonetheless, the concentration of $NH_4^+$ in the treated effluent appears to be particularly sensitive to the DO set-point, with a sharp increase happening at low DO levels. Regarding the $NO_3^-$ concentration in the treated effluent, the optimisation results suggest that the $NO_3^-$ concentration of less than 15 mg/l could be achieved through operational changes (increasing MLR and RAS flowrates), with no increase in the net energy consumption (compensated by a reduction of the compression energy). Reduction of the $NO_3^-$ concentration (down to 10 mg/l or lower) is also achievable by decreasing the solids capture in the primary sedimentation or further reduction of the $NO_3^-$ concentration (down to 5 mg/L or lower) is possible subject to an 18% increase in net energy consumption with addition of the external carbon source. The analysis of the second plant has mostly focused on the relationship between energy and effluent quality, using a systematic optimisation approach. An assessment of the overall environmental footprint would require that fugitive emissions are also taken into account in order to complete the picture.

### 8.1.2 Decision-making Tools for Sustainable Wastewater Treatment

The second contribution of the thesis was to develop a novel decision-making tool for the synthesis of sustainable wastewater treatment facility. The development of the decision-making tool is based on a superstructure optimisation approach for synthesis of wastewater treatment/resource recovery facilities using cutting-edge treatment and separation technologies to select the most promising system among hundreds or thousands of alternatives. A superstructure optimisation accounting for all process configurations is developed to determine the ideal network topology (treatment technologies, interconnections, and operating conditions) to maximise revenue or minimise the environmental footprint. However, with the current computational capabilities and available algorithms, solving the optimal design and operation of wastewater treatment systems in a single step is intractable due to complexity, multiple scales, time dependence, and uncertainty. The proposed methodology and key novelty relies on surrogate models as a means for overcoming the limitation of current global optimisation technology. A key requirement in applying this methodology nonetheless is the availability of reliable performance models for the treatment and separation units, on the one hand, and reliable costing and environmental impact data, on the other hand. This study advocates the use of state-of-the-art wastewater treatment simulators for deriving simple response-surface models, which are general enough to be independent of detailed design choices and keep the optimisation problem computationally tractable. Because such surrogate models may only provide an approximation of the actual performance and contain significant uncertainty, an iteration is typically required between the detailed process simulators and the superstructure-based optimisation problem to improve the surrogates' consistency and reliability. For those treatment/separation units that are a lack of reliable models or less well established, scenario-based analysis can be applied to predict performance and cost scenarios. The preselected plant configurations can be considered for detailed design analysis and optimisation in a subsequent step. The applicability of the proposed methodology has been presented through two case studies.

The first case study is the synthesis of a resource recovery facility based on industrial wastewater. It is relatively simple and limited to the wastewater stream. The results demonstate that the proposed methodology is computationally tractable using state-of-the-art optimisation technique that can provide a guarantee to global optimality. Also, the proposed framework can provide valuable insights for decision-making in WWTP design. The optimiser selects the resource recovery facility (UASB, Sand filtration, ion exchange and struvite crystalizer) as the optimal configuration to recover resources in terms of electricity, ammonia and struvite and provides sales revenue more than the OPEX. The extended superstructure optimisation framework to include biosolids management and to incorporate LCA with multi-objective optimisation is presented in the second case study. In this case, the synthesis of the municipal wastewater treatment facility was investigated to identify the trade-offs between conflicting objectives in terms of economic and environment. Our analysis has confirmed that the main trade-offs in terms of economic and environmental aspects can be captured. This would allow decision makers to be able to choose the most approapriate design based on their preference and balance between conflicting trade-offs. The results are presented as a set of the optimal solutions through a single and multi-objective optimisation, and that LCA integration into decision-making tools for wastewater treatment alongside economical considerations may lead to radical changes in the design of tomorrow's wastewater treatment facilities.

## 8.2 Future Directions

During the investigation of this study, some crucial points and discrepancies have been observed. As such, key recommendations for future studies are as follows:

### 8.2.1 Operational Considerations

Wastewater treatment is an energy intensive process. As discharge standards become stricter, energy use and fugitive emissions for WWTPs are likely to increase substantially. This study has highlighted that the use of plant-wide models to investigate different operational strategies can significantly improve operation of existing WWTPs in terms of effluent quality, energy use and fugitive emissions. Future works will focus on incorporation of biological/chemical phosphorus removal and GHG predictions into a systematic model-based optimisation approach to identify trade-offs between performance and the environmental criteria. The current plant-wide model for the systematic optimisation is based on BSM2 considering only carbon and nitrogen removal with one step nitrification/denitrification. Phosphorus removal is an important aspect to take into account because phosphorus is typically released in forms of phosphate under anaerobic conditions. Phosphorus removal requires large amount of energy in the activated sludge. In addition, more attention has been paid to GHG predictions, especially $N_2O$ in WWTPs. With capabilities of the systematic optimisation, trade-offs between standard regulations, energy consumption and fugitive emissions can be identified.

Another key study would be to extend a scenario-based robust optimisation problem to account for more uncertain parameters arisen from measurements and model parameters. Plant-wide models of WWTPs involve a number of uncertain parameters e.g. wastewater influent, kinetic and stoichiometric parameters in the models. It is important to account for uncertainty to improve insight into process behaviour to enhance model prediction accuracy and make solutions more practical. The variable interval optimisation approach, e.g. GlobSol software could be useful for this solving this problem. The optimal operational strategies will be assessed by simulating over uncertainty ranges based on the Monte Carlo (MC) approach to ensure that the certain operational strategies are flexible enough to satisfy with given uncertainty ranges. The MC method is commonly used for evaluating variations in the model predictions by sampling from the uncertainty ranges and propagating the sampled values through the model simulation to obtain a ranges of output values.

Based on the current plant-wide model, several assumptions have been made including a perfect plant-wide model with fixed model structure, parameters and fixed influent concentrations. This may contain inherent uncertainties and leads to the wrong conclusion. Although, the open-loop optimisation with the nominal values can provide the better understanding and improve performance of the wastewater treatment process, it is important to exploit the monitoring capacity and controllability to improve the accuracy and robustness of the model predictions. The model-based closed-loop optimal control can be a powerful for this problem and be a key extension for the future study. It is based on repeating the optimisation online through feedback of the measured variables. The control and operational strategies from the open-loop optimisation can be initially used to provide the optimal setting. Then, the measurement can provide new information about conditions and this enables the model to be updated (reduced model uncertainty). The optimisation can repeatly perform based on the updated model. Note that the current plant-wide model of the wastewater treatment process contains high non-linear terms and dimensional variables. Plant-wide model reduction could be used in this context.

### 8.2.2 Design Considerations

Synthesis of wastewater treatment/resource recovery facilities based on a superstructure-based optimisation is a promising approach towards sustainability. The ultimate goal of WWTPs is an energy-efficient process with a closed-cycle, where all wastewater is reused or recycled, and the only outputs of this process are saleable or value-added products. A key extension will be the development and regular update of information databases as new advanced treatment and recovery technologies develop, or as the economic, environmental and socio-cultural contexts evolve. Besides the availability of feasible technologies that can transform wastewater into a product, and the downstream processing of this product into a saleable item, the circumstances that are required to successfully establish a functioning and sustainable resource recovery system also involves developing a distribution infrastructure and catching investors' interest in developing such technologies.

Another future work would be to account for uncertainty in a superstructure-based optimisation model. Uncertainty in WWTP design is far less investigated than other process design fields and majority of the existing decision-making tools does not explicitly account for model robustness. Wastewater treatment is an inherently uncertain process due to large variation of wastewater influent. Instead of determining the optimal solution with nominal values, the optimisation formulation in presence of uncertainty aims to find the best possible solution with respect to the fact that all constraints with realisation of uncertainty are satisfied. A two-stage optimisation approach where the optimisation problem under uncertainty is divided into two sets could be employed. This approach is commonly used to include uncertainty into the decision-making process for the synthesis of chemical processes. The first stage involves selection of the decision variables before realisation of uncertainty. Subsequently, further design and operation can be improved when the uncertainty is taken into account.

Based on the proposed methodology, several software platforms are required to design the new wastewater treatment facility, e.g. GPS-X®, GAMS. However, it may not be convenient for a wide range of users and this may be the factors affecting the usability of the decision-making tool. A promising avenue would appear to be the development of an integrated and user-friendly platform for practical use. It is noted that several wastewater process simulators with a user-friendly interface and a wide library of treatment/separation units are already available. Thus, a key extension would be to integrate the proposed optimisation methodology within these wastewater process simulators, thereby making these tools widely available to decision-makers and practitioners.

# Chapter 9

# Example of gPROMS code [ASM1]

```
#Soluble inert organic matter                        SI     (1)
#Readily biodegradable substrate                     SS     (2)
#Particulate inert organic matter                    XI     (3)
#Slowly biodegradable substrate                      XS     (4)
#Active heterotrophic biomas                         XB,H   (5)
#Active autotrophic biomass                          XB,A   (6)
#Particulate products from biomass decay             XP     (7)
#Oxygen                                              SO     (8)
#Nitrate nitrite nitrogen                            SNO    (9)
#NH4   #+ + NH3 nitrogen                             SNH    (10)
#Soluble biodegradable organic nitrogen              SND    (11)
#Particulate biodegradable organic nitrogen          XND    (12)
#Alkalinity                                          SALK   (13)

Parameter
components  as    ORDERED_SET default     ['S_I','S_S','X_I','X_S','X_H','
   X_A','X_C','S_O','S_NO','S_NH','S_ND','X_ND','S_ALK']
y_a    as     real  default     0.24
y_h    as     real  default     0.67
f_p    as     real  default     0.08
i_xb   as     real  default     0.08
i_xp   as     real  default     0.06
mu_h   as     real  default     4
```

```
k_s    as    real  default     10
k_oh   as    real  default     0.2
k_no   as    real  default     0.5
b_h    as    real  default     0.3
n_g    as    real  default     0.8
n_h    as    real  default     0.8
k_h    as    real  default     3
k_x    as    real  default     0.1
k_nh   as    real  default     1
k_oa   as    real  default     0.4
k_a    as    real  default     0.05
T_as   as    real  default     14.8581
A      as    real  default     -66.7354
B      as    real  default     87.4755
C      as    real  default     24.4526
v      as    real
no_inlets    as    integer
no_outlets   as    integer
PORT
    inlet   as    array(no_inlets)   of    PMLMaterial DIRECTION_INLET
    outlet  as    array(no_outlets)  of    PMLMaterial DIRECTION_OUTLET

PORTSET
# Start Port Sets
    "inlet" as [inlet, outlet]
# End Port Sets

Variable
b_a          as          notype
y_h          as          notype
mu_a         as          notype
Q_in         as          array(no_inlets)              of     flowrate
Q_out        as          array(no_outlets)             of     flowrate
kla_ini      as          notype
u            as          array(no_inlets,components)   of     conc
```

```
rho          as        array(8)                     of    notype
rxn          as        array(components)            of    notype
y            as        array(components)            of    conc
mu_ht        as        notype
mu_at        as        notype
bht          as        notype
bat          as        notype
kat          as        notype
kht          as        notype
kla          as        notype
K            as        notype
T            as        notype
so_sat       as        conc


Equation
for i := 1 to no_inlets do
inlet(i).mass_flowrate        =     Q_in(i)                   ;
end
for i in components do
inlet().mass_fraction(i)      =     u(,i)                     ;
end
for i := 1 to no_outlets do
outlet(i).mass_flowrate =     Q_out(i)                  ;
end
# process aerobic tank
rho(1)       =     mu_ht*(y('S_S')/(k_s + y('S_S'))) * (y('S_O')/(k_oh + y('
    S_O'))) * y('X_H')   ;
rho(2)       =     mu_ht*(y('S_S')/(k_s + y('S_S'))) * (k_oh/(k_oh + y('S_O
    '))) * (y('S_NO')/(k_no + y('S_NO'))) * n_g * y('X_H')   ;
rho(3)       =     mu_at*(y('S_NH')/(k_nh + y('S_NH'))) * (y('S_O')/(k_oa +
    y('S_O')))  * y('X_A')   ;
rho(4)       =     bht*y('X_H')   ;
rho(5)       =     bat*y('X_A')    ;
rho(6)       =     kat*y('S_ND') * y('X_H')    ;
```

```
rho(7)      =     kht* y('X_S')/(y('X_H')+1e-6)/(k_x + (y('X_S')/(y('X_H')+1e-6))) * ((y('S_O')/(k_oh + y('S_O'))) + n_h * (k_oh/(k_oh + y('S_O')))* (y('S_NO')/(k_no + y('S_NO')))  ) * y('X_H') ;
rho(8)      =     kht* y('X_S')/(y('X_H')+1e-6)/(k_x + (y('X_S')/(y('X_H')+1e-6))) * ((y('S_O')/(k_oh + y('S_O'))) + n_h * (k_oh/(k_oh + y('S_O')))* (y('S_NO')/(k_no + y('S_NO')))  ) * y('X_H') * (y('X_ND')/(y('X_S')+1e-6)) ;



mu_ht =     mu_h * exp ((log(mu_h/3)/5) * (T_as - 15))  ;
mu_at =     mu_a * exp ((log(mu_a/0.3)/5) * (T_as - 15))  ;
bht   =     b_h * exp ((log(b_h/0.2)/5) * (T_as - 15))  ;
bat   =     b_a * exp ((log(b_a/0.03)/5) * (T_as - 15))  ;
kat   =     k_a * exp ((log(k_a/0.04)/5) * (T_as - 15))  ;
kht   =     k_h * exp ((log(k_h/2.5)/5) * (T_as - 15))  ;

# rxn aerobic tank
rxn('S_I')  =     0   ;
rxn('S_S')  =     - (1/y_h) * rho(1) - (1/y_h) * rho(2) + rho(7)    ;
rxn('X_I')  =     0   ;
rxn('X_S')  =     (1-f_p)* rho(4)  + (1-f_p)* rho(5) - rho(7)   ;
rxn('X_H')  =     rho(1) + rho(2) - rho(4)  ;
rxn('X_A')  =     rho(3) - rho(5)   ;
rxn('X_C')  =     f_p*rho(4) + f_p*rho(5)   ;
rxn('S_O')  =     -(1-y_h)/y_h * rho(1) - (4.57-y_a)/y_a * rho(3)  + kla * (so_sat - y('S_O'))  ;
rxn('S_NO') =     -(1-y_h)/(2.86*y_h) * rho(2) + 1/y_a * rho(3)   ;
rxn('S_NH') =     -i_xb * rho(1)  -i_xb * rho(2) - (i_xb + 1/y_a)*rho(3) + rho(6)    ;
rxn('S_ND') =     -rho(6) + rho(8)    ;
rxn('X_ND') =     (i_xb - f_p *i_xp)* rho(4) + (i_xb  - f_p * i_xp )* rho(5) - rho(8)    ;
rxn('S_ALK')      =     -i_xb/14 * rho(1) + ((1 - y_h)/(14*2.86*y_h) - i_xb/14)* rho(2) - (i_xb/14 + 1/(7*y_a))*rho(3) + 1/14 * rho(6)    ;
kla   =     (1.024^(T_as -15)) * kla_ini            ;
```

```
so_sat      =     0.9997743214 * 8 * 6791.5 * K/10.5           ;
K      =     56.12 * exp(A + B/T + C*log(T))    ;
T      =     (T_as + 273.15)/100                ;


for i in components do
$y(i) =     (1/v)*(SIGMA(inlet().mass_flowrate * inlet().mass_fraction(i))
    - SIGMA(outlet().mass_flowrate*y(i)) + v*rxn(i))    ;
end
SIGMA(outlet().mass_flowrate) =     SIGMA(inlet().mass_flowrate)   ;
#mass balance
for i in components do
outlet().mass_fraction(i)     =     y(i)                        ;
end
```

# Chapter 10

# Example of GAMS code

---

```
*Mass balance on source
eq1SO..
         Fin
                 =e=     sum(d_t,FIT(d_t)) + sum(d_j,FIE(d_j)) ;
*Mass balance on sink
eq2SI(d_j)..
         Fout(d_j)
                 =e=     FIE(d_j) + sum(d_t, FW(d_t,d_j)) + sum(d_t, FS(d_t
                    ,d_j))  ;
eq2_2SI(d_j,d_c)..
         Fout(d_j)*xout(d_j,d_c)
                 =e=     FIE(d_j)*xIN(d_c) + sum(d_t, FW(d_t,d_j)* xTUout(
                    d_t,d_c)) + sum(d_t, FS(d_t,d_j)* xWAS(d_t,d_c))  ;
*Mass balance on treatment unit
eq3TU(d_t)..
         FTUin(d_t)
                 =e=    FIT(d_t) + sum(d_tt, FTUW(d_tt,d_t)) +  sum(d_tt,
                    FTUS(d_tt,d_t))  ;
eq3_2TU(d_t,d_c)..
         FTUin(d_t)* xTUin(d_t,d_c)
                 =e=    FIT(d_t)*xIN(d_c) + sum(d_tt, FTUW(d_tt,d_t)*
                    xTUout(d_tt,d_c)) +  sum(d_tt, FTUS(d_tt,d_t)* xWAS(
```

```
                    d_tt,d_c))  ;
eq3_3TU(d_t)..
         FTUout(d_t)
                 =e=     sum(d_tt,FTUW(d_t,d_tt)) + sum(d_j,FW(d_t,d_j))   ;
eq3_4TU(d_t)..
         FTUwas(d_t)
                 =e=     sum(d_tt,FTUS(d_t,d_tt)) +   sum(d_j, FS(d_t,d_j))
                      ;
eq3_5TU(d_t)..
         FTUout(d_t)
                 =e=      FTUin(d_t)/FTUin_ref(d_t)*(sum(d_cc,mETF1(d_t,d_cc
                    )*xTUin(d_t,d_cc)) + bETF(d_t));
eq3_6TU(d_t)..
         FTUwas(d_t)
                 =e=      FTUin(d_t)/FTUin_ref(d_t)*(sum(d_cc,wETF1(d_t,d_cc
                    )*xTUin(d_t,d_cc)) + bwETF(d_t));
eq3_7TU(d_t,d_c)..
         xTUout(d_t,d_c)
                 =e=        sum(d_cc,mETx1(d_t,d_cc,d_c)*xTUin(d_t,d_cc))
                            + sum(d_cc,mETx2(d_t,d_cc,d_c)*power(xTUin(d_t,
                               d_cc),2))
                            + bETx(d_t,d_c)*yT(d_t);
eq3_8TU(d_t,d_c)..
         xWAS(d_t,d_c)
                 =e=        sum(d_cc,wETx1(d_t,d_cc,d_c)*xTUin(d_t,d_cc))
                            + sum(d_cc,wETx2(d_t,d_cc,d_c)*power(xTUin(d_t,
                               d_cc),2))
                            + bwETx(d_t,d_c)*yT(d_t);
```

# Chapter 11

# Example of Optimal Configurations for Multi-objective Optimisation

As presented in Chapter 6, multi-objective optimisation can be used to handle conflicting objective and a set of optimal solutions is generated in terms of Pareto-front. The results show that several optimal configuration can be obtained and the following process configurations are some examples of the optimal solutions shown on the Pareto-front.

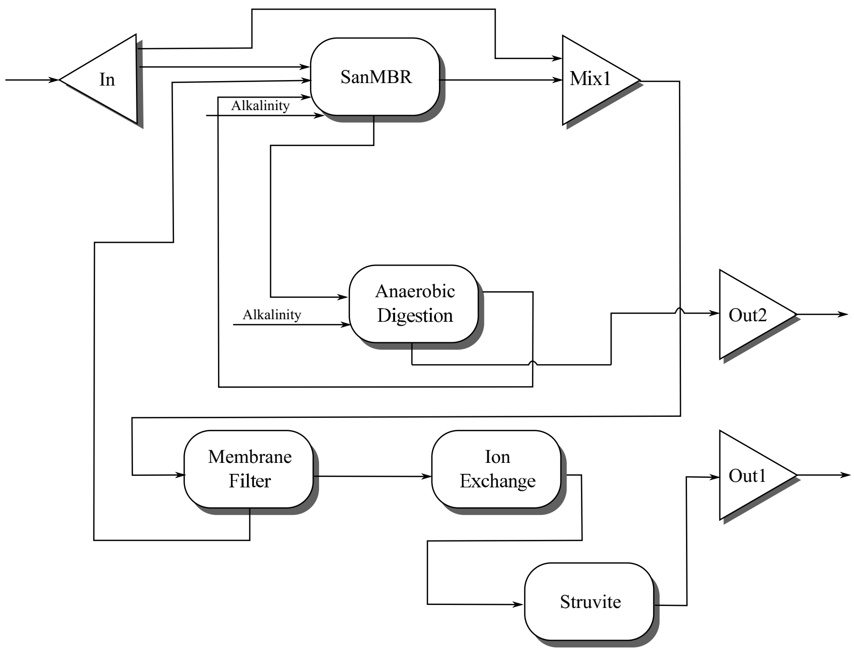



Figure 11.1: Example of the optimal configuration on the line A presented in Figure 6.10

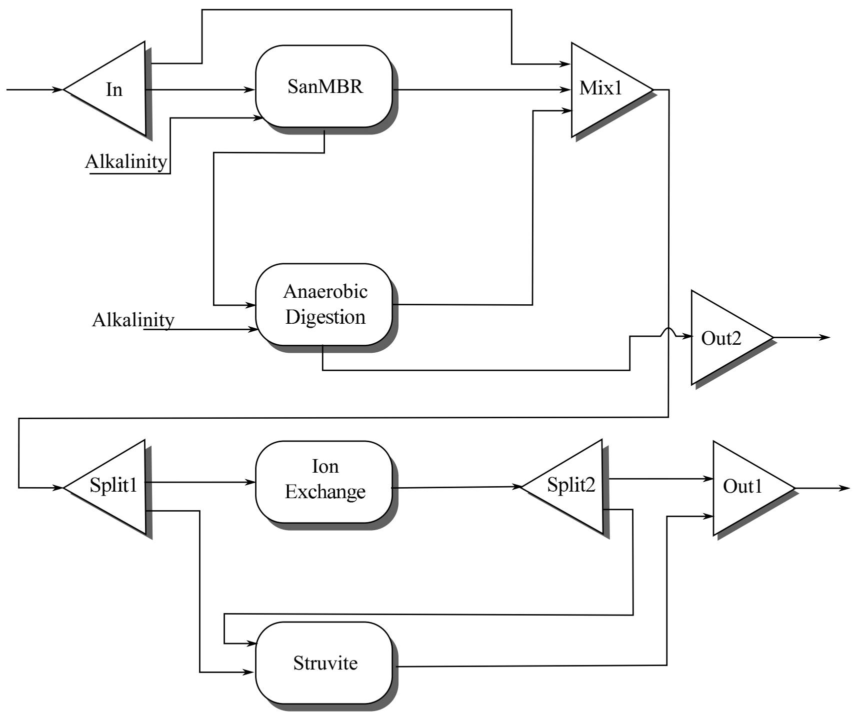



Figure 11.2: Example of the optimal configuration on the line B presented in Figure 6.10

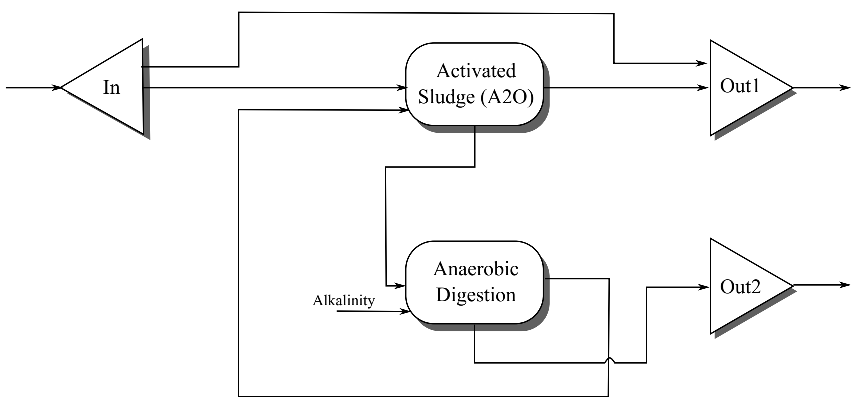



Figure 11.3: Example of the optimal configuration on the line C presented in Figure 6.10

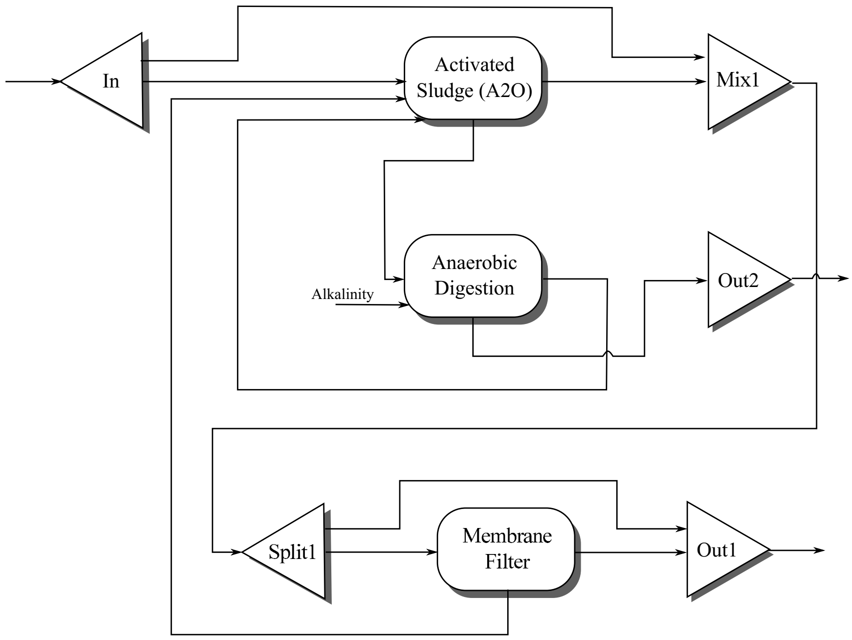



Figure 11.4: Example of the optimal configuration on the line C presented in Figure 6.10

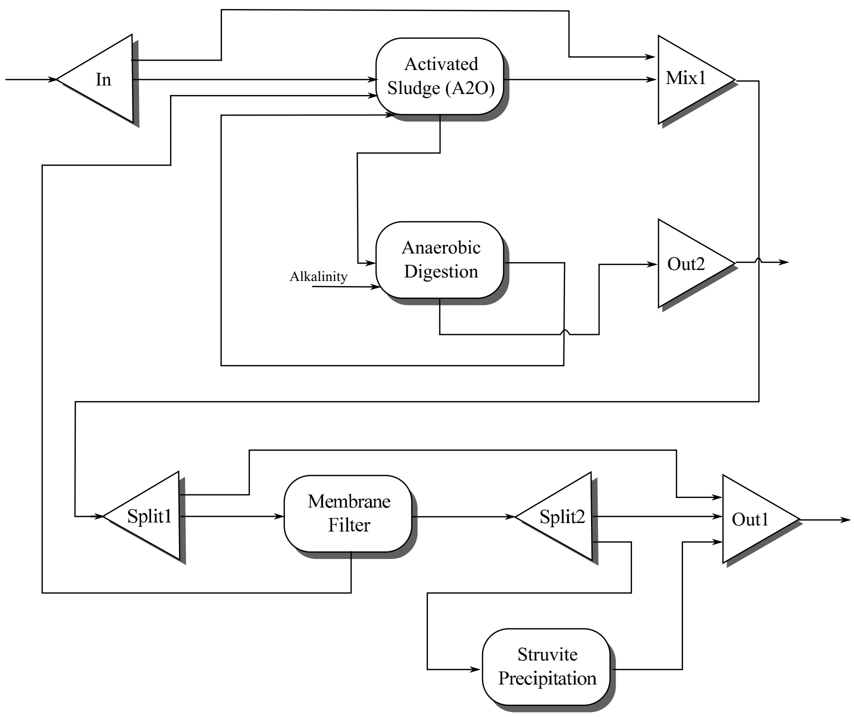



Figure 11.5: Example of the optimal configuration on the line C presented in Figure 6.10

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